

COALGEBRAIC BEHAVIOR ANALYSIS

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From Qualitative to Quantitative Analyses

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- [KK13] Henning Kerstan and Barbara König. Coalgebraic Trace Semantics for Continuous Probabilistic Transition Systems. *Logical Methods in Computer Science*, 9 [4:16](834), December 2013. doi:10.2168/LMCS-9(4:16)2013. arXiv:1310.7417v3 [cs.LO].

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- [BBKK15] Paolo Baldan, Filippo Bonchi, Henning Kerstan, and Barbara König. Towards Trace Metrics via Functor Lifting. In *6th Conference on Algebra and Coalgebra in Computer Science (CALCO’15)*. Lawrence S. Moss and Paweł Sobociński, editors. Volume 35. In Leibniz International Proceedings in Informatics (LIPIcs). Schloss Dagstuhl – Leibniz-Zentrum für Informatik, October 2015, pages 35–49. doi:10.4230/LIPIcs.CALCO.2015.35. arXiv:1505.08105 [cs.LO].

Moreover, Chapter 5 serves as a basis for an invited submission to a special issue of the journal *Logical Methods in Computer Science*.

Abstract

In order to specify and analyze the behavior of systems (computer programs, circuits etc.) it is important to have a suitable specification language. Although it is possible to define such a language separately for each type of system, it is desirable to have a standard toolbox that allows to do this in a generic way for various – possibly quite different – systems.

Coalgebra, a concept of *category theory*, has proven to be a suitable framework to model transition systems. This class of systems includes many well-known examples like *deterministic automata*, *nondeterministic automata* or *probabilistic systems*. All these systems are coalgebras and their behavior can be analyzed via the notion of final coalgebra or other category theoretic constructions.

This thesis investigates how to improve and build upon existing results to explore the expressive power of category theory and in particular coalgebra in behavioral analysis. The three main parts of the thesis all have a different focus but are strongly connected by the coalgebraic concepts used.

Part one discusses *adjunctions in the context of coalgebras*. Here, well-known automata constructions such as the powerset-construction are (re)discovered as liftings of simple and well-known basic adjunctions.

The second part deals with *continuous generative probabilistic systems*. It is shown that their trace semantics can be captured by a final coalgebra in a category of stochastic relations.

The final contribution is a shift from qualitative to quantitative reasoning. Via the development of methods to lift functors on the category of sets and functions to functors on pseudometric spaces and nonexpansive functions it is possible to define a *canonical, coalgebraic framework for behavioral pseudometrics*.

Preface

In this thesis I will present most of the results of four years of research which I conducted as a PhD student in the group of and under the supervision of *Barbara König* at the University of Duisburg-Essen. Before doing so, I would like to make some short remarks concerning the origins of this work as well as some personal comments.

Origins of the Material

The main chapters (Chapters 3 to 5) of this thesis are based on prior publications, which are the results of collaborations with other researchers. In all these collaborations, I contributed a lot to the development of the ideas. Moreover, the structure as well as the actual wording of the publications is to a major extent my own work. Due to this I took the liberty of including a lot of text verbatim from the referenced publications in the main chapters. However, whenever I considered it to be inappropriate (e.g., if a text part was entirely written by someone else and I had no part in it) I have either not included it or explicitly marked it or replaced the respective part of the text by a new one.

After these general remarks, I will now separately comment on the three main chapters and how they are related to the respective prior publications.

Adjunctions and Automata

The ideas connecting adjunctions and automata as presented in Chapter 3 arose out of discussions with several researchers. Together with *Barbara König* and *Bram Westerbaan*, I worked out the details of the theory, its application to examples and turned it into a conference paper [KKW₁₄]. Chapter 3 contains the results of this paper with the exception of the section on linear weighted automata, which was entirely Bram's work. I have added a few more examples to the main text and some additional proofs and calculations for this chapter can be found in Appendix A.1.

Trace Semantics for Continuous Probabilistic Transition Systems

The line of work on probabilistic systems presented in Chapter 4 has its roots in my diploma thesis [Ker11]. Together with *Barbara König*, I developed some non-trivial extensions of the results, which were then accepted as a conference paper [KK12b] and accompanied by a technical report [KK12a] containing the proofs. Later, in a special issue journal version [KK13], we integrated the proofs in the main text and demonstrated the theory on two sophisticated examples. Chapter 4 is based on this journal version.

In Appendix A.2 I have added a simpler proof of one of the results (measurability of the trace arrow) which was suggested to me by *Ernst-Erich Doberkat* after I presented this work on the Bellairs Workshop on Probability in 2014.

Behavioral Pseudometrics

The coalgebraic framework for behavioral pseudometrics as presented in Chapter 5 is a collaboration with *Paolo Baldan*, *Filippo Bonchi* and *Barbara König*. It is a combination of two consecutive conference papers [BBKK14; BBKK15]. The basis for Chapter 5 are the corresponding extended versions which are available online on arXiv.org but in contrast to them I have integrated the appendices with the proofs into the main text, added more explanations, improved several of the results and worked out more examples in detail.

As a last remark on this chapter, I would like to add that, after the second conference, we were invited to submit an article about our work on behavioral pseudometrics to a special issue of the journal *Logical Methods in Computer Science*. We will use this chapter as starting point for our submission.

Acknowledgements

While research is exciting and satisfying whenever one reaches a result (and even more so, if this result is accepted and honored by other scientists), the road to many of these results can be long and tedious. Fortunately there were many wonderful people who have supported and accompanied me on this road and who I want to mention here.

First of all, I would like to thank *Barbara König* for offering me the opportunity to pursue a PhD under her supervision. Conducting research together with her has always been an inspiring experience. She provided me with all the help I needed but also with a lot of freedom to develop and pursue my own ideas. Moreover, thanks to her I got to know many other researchers, was able to visit them and work with them.

The most inspiring and interesting aspect of science today are the international collaborations. Except from getting to know several nice and often sunny places, I met fascinating and extraordinary people all around the world.

Among these people, I will first mention my coauthors *Paolo Baldan*, *Filippo Bonchi* and *Bram Westerbaan*. It was and still is a pleasure not only to work with them but also to discuss everyday life topics while enjoying a good meal.

Another person I would like to thank here is *Alexandra Silva*. She rendered it possible to meet many other people of the coalgebraic community by inviting me to several workshops in Nijmegen, Braga and – together with *Prakash Panangaden* – to the Bellairs Research Institute on the amazing Caribbean island of Barbados.

Coming back from the Caribbean sea to Duisburg, I would also like to acknowledge my former and current colleagues *Harsh Beohar*, *Christoph Blume*, *Sander Bruggink*, *Mathias Hülsbusch*, *Dennis Nolte* and *Jan Stückrath* for interesting discussions and a good and friendly working environment.

A special thanks goes to my colleague *Sebastian Küpper* with whom I shared my office and thus naturally had a lot of interesting conversations. In particular, I am grateful for his helpful comments on many of my ideas including some early drafts of this thesis.

Another person I would like to mention here is *Tobias Heindel*. In the very beginning of my PhD, he invited me to a research visit to Paris and afterwards I met him at various conferences and workshops. On all these occasions, it was always interesting to discuss questions of science and everyday life.

Last but not least I would like to express my gratitude to those people who have played a significant part throughout my whole life and still continue to do that. I would not be who I am today, if it was not for the constant support I got and get from you, *my family* and *my friends*.

Duisburg, December 2015

Henning Kerstan

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Introduction

TRANSITION systems are one of the most fundamental structures of theoretical computer science. The underlying idea is that at every point in time a digital system like a circuit or a program is in a clearly defined state of a set of possible states and when time passes (in discrete time steps) the system can make a transition from one state to another. We assume that our model of such systems is *sequential*, i.e., we require that no transitions can occur simultaneously.

The most prominent examples of such transition systems are perhaps the well-known deterministic and nondeterministic finite automata which are used to describe and study regular languages but also other automata in the realm of formal languages like push-down automata or Turing machines are easily identified to have an underlying transition system structure. Apart from that, also process calculi like Robin Milner's *Calculus of Communicating Systems* (CCS) [Mil80] make use of transition systems: While syntactically a CCS-process is merely a word of a formal language, it induces a unique transition system which gives rise to its semantics.

The *behavior* of a transition system is defined in terms of the possible transitions between the states of the system. Depending on the respective system, such a transition can be labelled with an action which can represent a user input (e.g. pressing a button), an observable system output (a light or a display), a weight (a probability) or a condition (a switch) that has to be satisfied for the transition to be possible. In order to define the behavior of a system we usually assume that we can observe these outputs or interact with the system but we cannot see its internal state. Via the observations we make and the interactions that are possible, we can then compare any two systems and say if they behave similarly or not. Based on this, we can then characterize and analyze desired or wanted behavior, by first defining a transition system which serves as our *specification* and then comparing any given transition system to this specification to *verify* or *falsify* the implementation of the wanted behavior.

Any comparison as above induces in an apparent way a relation between transition systems. It is reasonable to assume that this relation is at least a

preorder: We want it to be *reflexive* so that each systems satisfies the specification given by itself and also to be *transitive* such that if system A satisfies the specification given by a system B which in turn satisfies the specification given by a system C we want the system A to satisfy the specification given by C. For our considerations we also require *symmetry*, i.e., we require that if a system A satisfies a specification given by B then this system also satisfies the specification given by A. This way we obtain an *equivalence relation* and thus a notion of equality (in terms of behavior) of transition systems.

A comparison of various notions of such behavioral equivalences for transition systems can be found in Rob van Glabbeek's seminal paper *The Linear Time – Branching Time Spectrum* [vGla90] along with an interpretation as *button pushing experiments*. In this thesis we will focus on the two extreme ends of that spectrum. We will consider the finest behavioral equivalence, *bisimilarity*, as well as the coarsest one, *trace equivalence*, using a (co)algebraic approach. Moreover, we will look into quantitative generalizations of both allowing us not only to say that two systems are different but also to quantify the extent of their difference.

1.1 Trace Equivalence versus Bisimilarity

Let us recall one standard example which demonstrates the weakness of trace equivalence and motivates bisimilarity. We imagine a vending machine offering two products: coffee and tea. In order to get a beverage, we have to first insert a coin and then choose which product we want. Thus the user actions are coin, coffee, and tea whereas the machine can react by serving tea or coffee, represented by the output actions $\overline{\text{tea}}$ or $\overline{\text{coffee}}$. If we just consider the linear behavior we want the machine to accept the sequences coin, coffee, $\overline{\text{coffee}}$ as well as coin, tea, $\overline{\text{tea}}$ but it should not accept sequences like coin, coffee, $\overline{\text{tea}}$ (wrong product served) or coin, coin, tea, $\overline{\text{tea}}$ (too much money payed) although the latter would be nice for the operator of the machine (or even necessary if the beverages' prices were very high). However, this specification by *traces* is not enough to get the desired result. Let us consider the two possible implementations given in Figure 1.1.1 which both satisfy our informal specification by traces given before.

We assume that both machines are in their top states (x_1 or y_1) in the beginning. The apparent difference is that the machine on the left hand side nondeterministically chooses which of the two transitions (to x_2 or to x_3) to take upon inserting a coin, so the user does not have a choice of a product any more! Contrary to that, the machine on the right hand side implements the correct behavior. In order to differentiate the two machines we will have to use

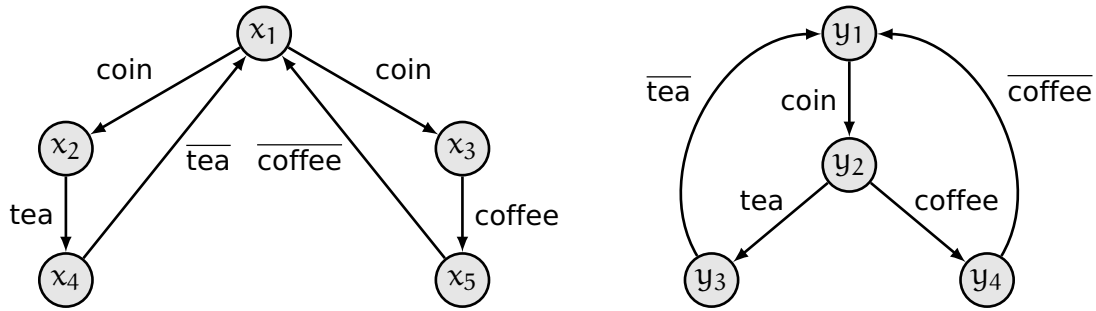


Figure 1.1.1: Two vending machines

an equivalence which is able to distinguish the *branching structure* of transition systems. This is where *bisimulations* come into play. We will not explain this important equivalence here but postpone its presentation to the Preliminaries (Chapter 2) since we need a formal definition of transition systems for this.

However, we will use the above example to point out one more thing. From the way we modelled our vending machines it is apparent that they *could* run forever, accepting e.g. infinite repetitions of the sequence coin, tea, $\overline{\text{tea}}$. While this is practically unlikely it is yet a sensible abstraction because we simply might not know how long the lifetime of such a vending machine will be. This complicates matters a bit because one can show that, even if we restrict our attention to the notion of traces, there are examples of transition systems which only differ in their infinite traces while agreeing on each finite one. In this thesis we will therefore consider both finite and infinite behavior.

1.2 Coalgebra as a Theory of Transition Systems

In recent years, the theory of coalgebras [JR97; Rut00] has proven to be a versatile tool that allows one to model and analyze various systems which are classically modelled as transition systems with possibly some side-effects like nondeterminism, probability or weights. The benefit of the coalgebraic view is that it provides the means for a uniform theoretic analysis of transition systems. While traditionally for each new transition system one has to define proper behavioral equivalences manually and argue why they are suitable, coalgebra provides a framework to do this in a canonical fashion.

Although coalgebra is a concept of category theory [Mac98] which is highly non-trivial and requires a lot of time to be understood properly, the basic ideas of coalgebra can be understood very quickly by looking at familiar examples.

Let us, for instance, consider a deterministic finite automaton (DFA). It is

classically modelled as a quintuple (X, A, x_0, δ, F) where X is a finite set of states, A is a finite alphabet (regarded as inputs of the automaton), $x_0 \in X$ is the initial state, $\delta: X \times A \rightarrow X$ is the transition function and $F \subseteq X$ is a set of final states. Such an automaton starts in its initial state x_0 and then, depending on the given input signals, it changes its state according to the transition function until it reaches a final state $x_f \in F$. We think of it as accepting the word that is obtained by concatenating the input signals that steered the automaton from its initial state to the final state.

The important thing to notice is that the *dynamics* of the system is entirely given by the transition function. If instead of the above function we had a function $\delta: X \times A \rightarrow \mathcal{P}X$, where $\mathcal{P}X$ denotes the set of all subsets of X , we would obtain¹ a nondeterministic finite automaton (NFA). Similarly, probabilistic automata are essentially defined by a transition function of the form $\delta: X \times A \rightarrow \mathcal{D}X$. Here $\mathcal{D}X$ is the set of all probability distributions on X , i.e., the set of all functions $p: X \rightarrow [0, 1]$ such that $\sum_{x \in X} p(x) = 1$. Thus the transition function δ of a probabilistic automaton maps each state $x \in X$ and each input $a \in A$ to the distribution $\delta(x, a): X \rightarrow [0, 1]$. The underlying intuition is, that if such an automaton is in state x it reacts to the input a by choosing a successor state $x' \in X$ according to the probabilities given by $\delta(x, a)$.

Keeping the above observation in mind, it thus seems plausible to focus on the transition structure of systems which is exactly what coalgebra does. If we restrict our attention to the realm (or more precisely the *category*) of sets and functions, a coalgebra is nothing but a function of shape $X \rightarrow FX$ where F is a so-called functor, i.e., a special higher order function that maps sets to sets and functions to functions. This functor F determines the branching type of the system. For instance, deterministic automata can be modelled as functions $c = \langle o, s \rangle: X \rightarrow 2 \times X^A$ where $2 = \{0, 1\}$ and X^A is the set of all functions from A to X . Each state $x \in X$ gets assigned a value $o(x) \in 2$ determining whether it is final ($o(x) = 1$) or not ($o(x) = 0$) and a successor function $s(x): A \rightarrow X$. To see that this is indeed a coalgebraic model of a deterministic automaton we just have to remind ourselves that via currying/uncurrying the function $s: X \rightarrow X^A$ can equivalently be expressed as function $\delta: X \times A \rightarrow X$ and vice versa. Moreover, one can indeed extend the function mapping the set X to the set $2 \times X^A$ to a functor. In a similar way, nondeterministic automata can be modelled as coalgebras $X \rightarrow 2 \times (\mathcal{P}X)^A$ and probabilistic automata are coalgebras $X \rightarrow 2 \times (\mathcal{D}X)^A$.

The above examples provide already a small insight into the expressive power

¹If we wanted to be very precise, we would also have to replace the initial state x_0 by a set of initial states $I \subseteq X$.

of coalgebra and it should be imaginable that the definition is flexible enough to encompass many more types of (labelled) transition systems. All we have to do is to tweak our sole parameter – the functor F . Such a functor cannot only be defined on the category of sets and relations as above but also on other categories like the category of sets and *relations*. As simple example for this we observe that the transition function $\delta: X \times A \rightarrow \mathcal{P}X$ of a nondeterministic automaton can equivalently be characterized by a *relation* $R \subseteq X \times A \times X$ if we define $R := \{(x, a, x') \mid x' \in \delta(x, a)\}$.

Before continuing, we quickly point out a subtle peculiarity. When we look again at the above coalgebras we can see that we have simply integrated the notion of final state into the coalgebra. However, initial states are not part of the coalgebra. This is not a mistake but it is common for the coalgebraic modelling and we will discuss this issue in some more details once we have provided the basic definitions in the Preliminaries (Chapter 2).

Let us now emphasize that coalgebra not only allows to *model* systems in a unified way but also permits to *define and analyze their behavior*. The key to this behavioral analysis is the observation that for some functors there exist special coalgebras – so-called *final* coalgebras – which have the property (and are defined uniquely via it) that every system has a unique mapping into it.

As example we remark that the set $\mathcal{P}(A^*)$ of all languages over A is a deterministic (but unless $A = \emptyset$ certainly not finite) automaton. Its final states are all the languages containing the empty word ε and for every state (a language) L its a -successor is the a -derivative of L , i.e., the language $L_a := \{aw \mid w \in L\}$. Thus we also have a coalgebra of all languages $z: \mathcal{P}(A^*) \rightarrow 2 \times (\mathcal{P}(A^*))^A$. This coalgebra is the final coalgebra for the underlying functor. For any other deterministic automaton represented as a coalgebra $c = \langle o, s \rangle: X \rightarrow 2 \times X^A$, we have a unique function $\llbracket \cdot \rrbracket: X \rightarrow \mathcal{P}(A^*)$ mapping each state $x \in X$ to the language it accepts. Since language equivalence and bisimilarity coincide for deterministic systems, this map yields both of these notions: Two states x and y are bisimilar (and apparently language equivalent) if and only if they are mapped to the same state (language) in the final coalgebra, i.e., if $\llbracket x \rrbracket = \llbracket y \rrbracket$.

We will later see that the behavioral equivalence which is induced by the map into the final coalgebra in general corresponds to bisimilarity. It is thus finer than language equivalence unless they coincide as in the example above. If we now turn our attention to nondeterministic automata we are hence faced with two challenges. On the one hand we will see that the final coalgebra for these automata does not exist (we would have to restrict our attention to finitely branching systems) and on the other hand if we are interested in the coarser language equivalence, we will have to dig deeper into the coalgebraic theory to find a satisfying answer.

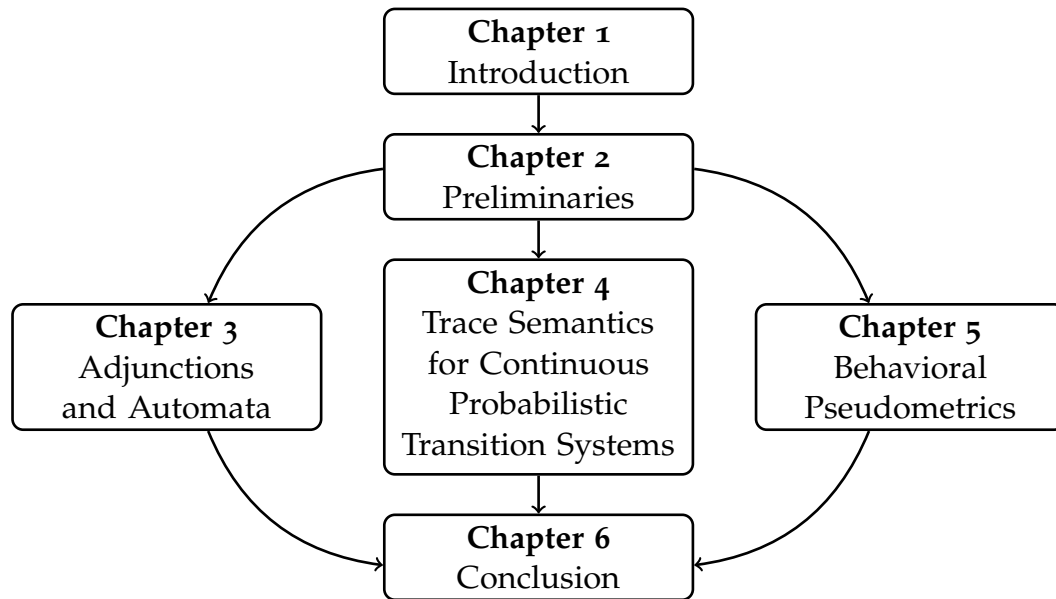


Figure 1.3.1: Interdependencies of the chapters. An arrow indicates that the chapter at the source of the arrow is a prerequisite of the chapter at the arrow tip.

1.3 Structure of the Thesis

Equipped with at least the basic, example-guided understanding of coalgebra from above we can now discuss the structure of this thesis and its contributions. Its general aim is to continue the analysis of the expressive power of coalgebraic methods in the analysis of labelled transition systems. This is done in a total of six chapters whose interdependencies are depicted in Figure 1.3.1.

Apparently, the current introductory chapter serves to identify the coalgebraic behavioral analysis as overall topic of the thesis. Moreover, it is intended as a guide for the reader to understand the modular structure of this thesis.

The three main chapters (Chapters 3 to 5) are completely independent of each other and can be read separately in any order. However, they share a common mathematical background which is presented in Chapter 2.

A lot of effort has been put already into this mathematical background in Chapter 2 to make it in principle possible to read this thesis without any prior knowledge of category theory or coalgebra. Therefore, this chapter takes the reader through a short but concise tour of all the basics from category theory, transition system theory and coalgebra commonly needed for the later parts of this thesis. Moreover, it always provides references to the literature where the corresponding concepts are explained in more details.

Of course, readers who are familiar with category theory and coalgebra can skip this part but are nevertheless advised to at least give it a quick look because all notational conventions will also be explained there. However, there is a quite extensive List of Symbols and an Index at the end of the thesis so it is also possible to look up the notation only when needed.

The thesis ends with a short chapter containing some concluding remarks in Chapter 6. As visible in the diagram of Figure 1.3.1, these require the knowledge of all main chapters.

1.4 Contributions

The contributions of this thesis are split into three chapters (Chapters 3 to 5) which all have a similar basic setup. Each of them starts with an introductory text explaining in more details the contributions of the chapter. While Chapter 3 does not require any additional mathematical background, Chapters 4 and 5 do, so the introductory text is succeeded by a section explaining further mathematical preliminaries, which are just relevant for the respective chapter. All three chapters end with a separate conclusion section in which their respective contributions are summarized and put into the larger research context.

In the subsequent overview of these three chapters we will already use some of the terminology and notation which is explained only later in the Preliminaries (Chapter 2). However, even with just the ideas from above it should be possible to get a general understanding of what will happen in the chapters.

Chapter 3. Adjunctions and Automata

This chapter is a case study looking into adjunctions – one of the important abstract concepts of category theory – in the context of several automata models which are, of course, represented as coalgebras.

In order to get an idea of adjunctions, let us consider a standard example which is easily understandable. We first recall that for any set A the set A^* consists of all the finite words (also called strings or lists) of elements of A . We can append a word v to another word w yielding the word wv which gives rise to a concatenation operation $\text{conc}: A^* \times A^* \rightarrow A^*$ where, of course, $\text{conc}(w, v) = wv$. This operation is *associative*² and the empty word ε serves as both-sided *neutral element*³. Any set M together with such an associative

²For all $w_1, w_2, w_3 \in A^*$ we have $(w_1 w_2) w_3 = w_1 (w_2 w_3)$.

³For all words $w \in A^*$ we have $w\varepsilon = \varepsilon w = w$.

operation $\circ: M^2 \rightarrow M$ and a both-sided neutral element $e \in M$ is called a *monoid* and our monoid A^* is given the special name *free monoid* because it satisfies a so-called *universal property*: For any monoid (M, \circ, e) there is a bijection between functions $f: A \rightarrow M$ and monoid homomorphisms⁴ $h: (A^*, \text{conc}, \varepsilon) \rightarrow (M, \circ, e)$ satisfying $h(a) = f(a)$ for all $a \in A$. Explicitly, given a function f as above and any string $a_1 \dots a_n$ we define $h_f(a_1 \dots a_n) = f(a_1) \circ \dots \circ f(a_n)$ and conversely for any monoid homomorphism h as above and any element $a \in A$ we define $f_h(a) = h(a)$. Thus we can think of the free monoid construction as the *most efficient way* to turn an arbitrary set into a monoid which includes that set.

In category theory this observation is formalized by the notion of *adjunction*. The function mapping a set to its free monoid can easily be extended to a functor (we just have to define how it transforms functions into monoid homomorphisms between free monoids) and apparently we can map any monoid to its underlying set and a monoid homomorphism to the underlying function which gives rise to another functor. Due to the above bijection we say that these two functors are *adjoint*. We will explain this more thoroughly in Section 2.3.4.

In Chapter 3 we look at the well-known powerset construction which transforms a nondeterministic automaton into an equivalent deterministic one from a categorical perspective. It turns out that this construction is a functor which happens to be the right adjoint to the inclusion functor from a category of deterministic automata to a category of nondeterministic automata.

Since automata are coalgebras, this is just an adjunction between two categories of coalgebras: we consider deterministic automata as coalgebras in *Set* and nondeterministic automata as coalgebras in *Rel*. Looking closely, one can see that this adjunction between coalgebras arises out of a canonical adjunction between the categories *Set* and *Rel*.

Taking this observation as leading idea, we first identify generic sufficient conditions to lift an adjunction between two categories to an adjunction between coalgebras for functors on these categories. Moreover, we compare our conditions with a more general 2-categorical result.

Afterwards we illustrate the applicability of this lifting technique in length. While doing so, we recover several constructions on automata as liftings of well-known basic adjunctions including

- ▷ the determinization of nondeterministic automata via the well-known powerset construction,
- ▷ a similar construction we call *codeterminization*, which transforms a nondeterministic automaton into a backwards deterministic automaton where each

⁴A monoid homomorphism between two monoids (M, \circ, e_M) and $(N, *, e_N)$ is a function $h: M \rightarrow N$ such that $h(e_M) = e_N$ and $h(m_1 \circ m_2) = h(m_1) * h(m_2)$ for all $m_1, m_2 \in M$.

state has a unique predecessor for each action symbol, and

- ▷ determinization of *join-automata*, a special class of automata whose state space is a complete join semi-lattice and whose transition function respects this structure.

As a final contribution, we show how the lifted adjunction can be used to check behavioral equivalences. Proofs and some additional calculations are provided in Appendix A.1.

Chapter 4. Trace Semantics for Continuous Probabilistic Transition Systems

As we have briefly discussed in the beginning, the behavioral equivalence induced by the unique map into the final coalgebra is bisimilarity. Obtaining the coarser notion of trace equivalence coalgebraically is possible but requires a bit more effort.

In order to do so, let us first take a brief look at so-called *monads* and then discuss how such a monad can be used to obtain traces. By reviving our example of the free monoid construction which we used before to look at adjunctions, we can also get an idea of a monad⁵. In presence of the free monoid A^* of a set A there are two useful functions. First of all, there is the apparent inclusion $\eta_A: A \rightarrow A^*$ mapping an element $a \in A$ to itself interpreted as a one element word or string. If we denote each element $w \in A^*$ by enclosing them in quotation marks we can thus write $\eta_A(a) = "a"$. Secondly, we have a function $\mu_A: (A^*)^* \rightarrow A^*$ which maps a list of words to the word we obtain by concatenating all the words. Employing the quotation mark notation we have $\mu_A(("w_1" "w_2" \dots "w_n")) = "w_1w_2 \dots w_n"$ for all $w_1, w_2, \dots, w_n \in A^*$. Moreover, for any function $f: A \rightarrow B$ we can define a function $f^*: A^* \rightarrow B^*$ by requiring $f^*("a_1a_2 \dots a_n") = "f(a_1)f(a_2) \dots f(a_n)"$. This yields a functor T on the category of sets and functions. The aforementioned functions and this functor satisfy certain compatibility laws which is the reason why we call the triple (T, η, μ) the *list monad*. In fact, one can show that this notion coincides with the monads used in functional programming languages such as Haskell. As in these languages the strength of monads in the coalgebraic treatment of transition systems is that they allow to hide side-effects in the branching structure. Thus we can specify which branching is important (e.g. the user input or the system output) and which branching can be condensed (e.g. nondeterministic or probabilistic branching) for the behavioral analysis.

An approach by Ichiro Hasuo, Bart Jacobs and Ana Sokolova [HJS06] suggests

⁵This is not a coincidence. In fact, we will see in Chapter 2 that monads and adjunctions are closely connected.

to interpret systems which are coalgebras of the shape $X \rightarrow TFX$ where F is an endofunctor and (T, η, μ) a monad on Set as coalgebras in the Kleisli-category of the monad. In there, the above coalgebra corresponds to a coalgebra $X \rightsquigarrow \widehat{F}X$ for an extension \widehat{F} of the original functor. If this functor admits a final coalgebra, it gives rise to a notion of trace semantics which we will explain in Section 2.4.3.

The aforementioned approach encompasses a class of discrete probabilistic systems which is slightly different from the probabilistic automata in the beginning. Such a *generative* probabilistic transition system is a coalgebra $c: X \rightarrow \mathcal{D}(A \times X + \mathbb{1})$ in Set and it can be interpreted as a probabilistic generator for words. Whenever it is in a state $x \in X$ it can either move with output $a \in A$ to a state x' and does this with probability $c(x)(a, x') \in [0, 1]$ or it can terminate and does this with probability $c(x)(\checkmark)$ with \checkmark being the unique element of the singleton $\mathbb{1}$. For each state $x \in X$ of such a system its trace is a probabilistic language, i.e., a probability distribution $\text{tr}(x): A^* \rightarrow [0, 1]$ which arises as the unique Kleisli-arrow into the final coalgebra of the lifted functor.

In the above model of discrete probabilistic systems the support of the respective distributions is at most countable. As we will see in Chapter 4, this not only excludes several interesting examples but it also prevents a treatment of infinite traces since the set of infinite words A^ω is uncountable. In order to treat them properly, it is necessary to use concepts from measure theory.

In Chapter 4 we thus generalize the above approach for a coalgebraic definition of traces to generative probabilistic transition systems, with arbitrary (possibly uncountable) state spaces. We do so by moving to the category Meas of measurable spaces and functions where we consider suitable generalizations of the functors from above.

On this category, there are two known probabilistic monads, the sub-probability monad and the probability monad (Giry monad). Our main technical contribution is that the existence of a final coalgebra in the Kleisli category of these monads is closely connected to the measure-theoretic extension theorem for sigma-finite pre-measures.

As a concrete result, we obtain a practical definition of the trace measure for both finite and infinite traces of arbitrary generative probabilistic systems which extends the result for discrete systems. In order to demonstrate the applicability of our result, we finally consider two example systems with uncountable state spaces and calculate their trace measures.

Chapter 5. Behavioral Pseudometrics

Especially in the presence of quantitative information like probabilities or other numerical weights, it seems too strict to require that two states of a system

behave *exactly* the same.

Let us elaborate on this by considering the probabilistic system depicted below in Figure 1.4.1 (taken from [vBW06]). It is a purely probabilistic transition system with state space $X = \{u, x, y, z\}$ and an arbitrary $\varepsilon \in]0, 1/2[$. The intuitive understanding of such a system is, that in each state the system chooses a transition (indicated by the arrows) to another state using the probabilistic information which is given by the numbers on the arrows.

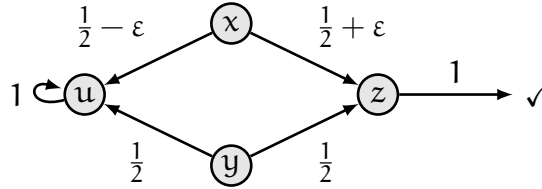


Figure 1.4.1: A probabilistic transition system

The state z on the right hand side is a *final state* so the system terminates with probability one (indicated by the arrow to \checkmark) when reaching that state. Contrary to that, state u on the left hand side can be interpreted as a *fail state* which – once reached – can never be left again and the system loops indefinitely in u . Thus the behavior of these states is entirely different. If we now compare the other two states x and y in this system it should be obvious that they are *similar* for a small ε . However, unless ε is 0 (which we disallow), they will never behave exactly the same, because in state x it is always a little bit more probable to go to state z instead of u .

A situation as in this toy example could for instance arise, if the probabilities come from (imprecise) measurements or simply if we have numerical errors when implementing such a system using floating point calculations.

An obvious solution for our above problem is to consider behavioral distances instead of behavioral equivalences. In this setting, we simply say that x and y are ε apart (they are indeed if we take the proper behavioral distance) and whenever ε is small enough, we might be satisfied with that.

In order to obtain such distances for probabilistic systems there are at least three different possibilities:

- ▷ Firstly, one can consider ε -bisimulations, a quantitative variant of (probabilistic) bisimulation and then define the distance of two states to be the smallest ε such that they are ε -bisimilar (and 1 if they are not bisimilar) [GJS90].
- ▷ Secondly, we note that probabilistic bisimulation can be captured using a simple modal logic without negation in the sense that two states are bisimilar if and only if they satisfy the same formulae [DEP98]. Using a continuous

evaluation of these formulae, allowing real truth values ranging from 0 to 1, one can then define a distance by taking the largest difference of these evaluations [DGJP99].

- ▷ Finally, using ideas from transportation theory [Vil09] it is possible to define a distance as a fixed point of an equality which relies on a *lifting* of distances on X to the set $\mathcal{D}X$ of distributions on it [vBW06].

While the latter two approaches already use a coalgebraic framework, up until now they are specific to the probabilistic setting. In Chapter 5 we generalize the third approach to study behavioral metrics in an abstract coalgebraic setting. Given a coalgebra $c: X \rightarrow FX$ in \mathbf{Set} we define a framework for deriving pseudometrics on X which measure the behavioral distance of states.

A first crucial step is the lifting of the functor F on \mathbf{Set} to a functor \bar{F} in the category \mathbf{PMet} of pseudometric spaces. We present two different approaches which can be viewed as generalizations of the Kantorovich and Wasserstein pseudometrics for probability measures. We show that the pseudometrics provided by the two approaches coincide on several natural examples, but in general they differ.

Using the above lifting, a final coalgebra for an endofunctor F on \mathbf{Set} can be endowed with a behavioral distance resulting as the smallest solution of a fixed-point equation, yielding the final \bar{F} -coalgebra in \mathbf{PMet} . The same technique, applied to an arbitrary coalgebra $c: X \rightarrow FX$ in \mathbf{Set} , provides a canonical behavioral distance on X . Under some constraints we can prove that two states are at distance 0 if and only if they are behaviorally equivalent.

As in the case of behavioral equivalences, the above approach yields bisimilarity distances and it requires some additional effort to define trace distances. We will obtain them by combining our framework with the so-called generalized powerset construction [SBBR10].

This construction was suggested by Alexandra Silva, Marcello Bonsangue, Filippo Bonchi and Jan Rutten as another approach to coalgebraic trace semantics. It works for coalgebras $c: X \rightarrow FTX$ on \mathbf{Set} where F is an endofunctor and (T, η, μ) is a monad and requires a certain distributive law $\lambda: TF \Rightarrow FT$. The basic observation is, that this distributive law induces a generic determinization construction which transforms the above FT -coalgebra into a \hat{F} -coalgebra for a lifting \hat{F} of F to the Eilenberg-Moore category of the monad. We can then embed the original system in its determinization using the unit η of the monad. Moreover, a final F -coalgebra induces a final \hat{F} coalgebra which can then be used to obtain trace semantics via finality.

In order to apply this construction in our setting, we generalize our technique for systematically lifting functors from the category \mathbf{Set} of sets to the category

PMet of pseudometric spaces, by identifying conditions under which also natural transformations, monads and distributive laws can be lifted.

If we are in such a setting, i.e., if we have a coalgebra $c: X \rightarrow FTX$ and a distributive law $\lambda: TF \rightarrow FT$ such that the functor, the monad and this law can be lifted to PMet and F has a final coalgebra we obtain trace semantics as follows.

- ▷ First, we determinize the Set-coalgebra using the generalized powerset construction in Set,
- ▷ then we equip the final F -coalgebra with its behavioral distance using our lifting framework from above and
- ▷ finally we define the distance of two states to be the behavioral distance of their image in the determinization via the unit of the monad.

Of course we also demonstrate how to use this procedure to obtain trace distances for nondeterministic and probabilistic automata.

Summing up, this last chapter provides a generic, coalgebraic approach to behavioral pseudometrics for all transition systems which can be modelled as coalgebras in the category of sets and functions. Thus whenever we devise a new type of transition system, it is now possible not only to automatically obtain canonical behavioral *equivalences* in a unified way but also behavioral *pseudometrics* which extend these equivalences in the sense that equivalent states have distance 0.

Preliminaries

AN important part of research is to communicate one's own findings to other researchers. In order to succeed, it is crucial to agree upon a common *basic knowledge*.

Since this thesis combines several areas of computer science and mathematics, the purpose of this chapter is to provide the basic knowledge needed to understand the results in the main parts of this thesis. However, it is of course impossible to explain every bit of it so one has to rely on some assumptions. The assumption made here is that the reader has a thorough mathematical and computer science background (roughly at the level of an undergraduate degree at a university). It is intended that the results in this thesis in principle are accessible to anyone satisfying these minimal prerequisites although it will most likely require some effort.

Readers who are familiar with the presented topics can of course skip this chapter, immediately move on to (one of) the main parts of the thesis and just consult this chapter whenever they are in need of an explanation. It should be possible to quickly find definitions or notations by consulting the List of Symbols or the Index.

2.1 Foundation

When starting to learn mathematics, one usually relies on an intuitive understanding of both propositional and predicate logic. This works quite well because for many areas of mathematics such a basic understanding is sufficient. The same holds true for one of the most fundamental structures in mathematics: the notion of a *set*.

2.1.1 Set Theoretic Assumptions

A common naive understanding is that, given any “property” (e.g. a unary predicate) Φ the “elements” satisfying this predicate constitute a set $\{X \mid \Phi(X)\}$.

This understanding yields to the following, well-known paradox, which is commonly attributed to Bertrand Russell. Suppose we wanted to define a set whose elements are themselves sets. Let $\Phi(X)$ denote the property that $X \notin X$, i.e., that the set X is not an element of itself. Then the set $R := \{X \mid \Phi(X)\} = \{X \mid X \notin X\}$ of sets not containing themselves is properly defined according to the intuitive understanding of a set. However, since R is itself a set, we may ask whether R is an element of R . This leads to the contradiction $R \in R \iff R \notin R$.

The problem that leads to this contradiction is the principle of *unrestricted comprehension*, i.e., the idea that *every* property defines a set.

In order to avoid such problems, we will abandon the naive set theory and work in a more rigorous, axiomatic set theory. For our purposes we thus assume some set-theoretic foundation including the notion of (*proper*) *classes*, i.e., entities that might be too large to be a set and sometimes even (possibly) larger entities, called *conglomerates* (see e.g. the “Joy of Cats” textbook [AHS90, p.13ff] for a detailed discussion of their properties). These notions form a (strict) hierarchy, i.e., any set is a (non-proper) class but there are classes which are not sets (the obvious example being the class of all sets) and similarly any class is a conglomerate but there are conglomerates which are not classes (like the conglomerate of all classes).

This formal setup can be achieved by requiring e.g. the von-Neumann-Bernays-Gödel (NBG) axioms or the Zermelo-Fraenkel (ZFC) axioms and a universe axiom in the style of Grothendieck (see e.g. [Gab62; Mac69] for more details on universes). In any case we do assume an *axiom of choice* (although we won’t usually make explicit use of it). In the remainder of this section we will first introduce our notation for logical connectives, sets, classes and conglomerates and constructions with them. The existence of the respective entities has to be provided by our axiomatic (set theoretic) foundation.

2.1.2 Notation and Basic Definitions

For logical statements we will employ the symbols \wedge (*conjunction/and*), \vee (*disjunction/or*), \implies (*implication*), \iff (*biconditional, bi-implication*), \exists (*existential quantification*) and \forall (*universal quantification*).

The *membership relation* of sets, classes (and even conglomerates, where applicable) will all be denoted by the usual symbol \in , i.e., we write $x \in X$ to indicate that x is an element of the set (or the class, or even the conglomerate) X and the negation of membership is indicated by the symbol \notin . For sets (or classes or conglomerates) X, Y we write $X = Y$ for equality, $X := Y$ for assignment (equality by definition), $X \subset Y$ for strict inclusion and $X \subseteq Y$ for non-strict inclusion. Their negation is denoted by the symbols \neq , $\not\in$ or $\not\subseteq$ respectively.

The unique *empty set*, i.e., a set without any element, is denoted by the symbol \emptyset . By $\mathbb{1}$ we denote a *singleton* set and its unique element usually by \checkmark . Similarly we write $\mathbb{2}$ for a two element set whose elements are (if not specified otherwise) the integers 0 and 1.

Let for the remainder of this paragraph X and Y be classes. We write $\mathcal{P}X$ or $\mathcal{P}(X)$ for the *power class* of X , i.e., $\mathcal{P}X = \{S \mid S \subseteq X\}$. For *relative complements* we write $X \setminus Y$, i.e., $X \setminus Y = \{x \in X \mid x \notin Y\}$, for the *intersection* $X \cap Y = \{z \mid z \in X \wedge z \in Y\}$ and for the *union* $X \cup Y = \{z \mid z \in X \vee z \in Y\}$.

The *cartesian product* $X \times Y$ is the class $\{(x, y) \mid x \in X \wedge y \in Y\}$ of ordered pairs which we write using parentheses (the same applies to other tuples).

The *disjoint union* $X + Y$ formally is the class $\{(x, 0), (y, 1) \mid x \in X, y \in Y\}$. If X and Y are *disjoint*, i.e., $X \cap Y = \emptyset$, the disjoint union coincides with (is isomorphic to) the usual union $X \cup Y$ in an obvious way. We will often silently assume that this is the case and write e.g. $x \in X + Y$ instead of $(x, 0) \in X + Y$.

We call any subclass $R \subseteq X \times Y$ a (*binary*) *relation* (from X to Y) and similarly if Z is another class we call $R \subseteq X \times Y \times Z$ a *ternary relation*. For binary relations we write xRy instead of $(x, y) \in R$.

If a binary relation $f \subseteq X \times Y$ satisfies the requirement that for any $x \in X$ there is a unique $y \in Y$ with $(x, y) \in f$ we call it a *function* (with *domain* X and *codomain* Y), denote it by $f: X \rightarrow Y$ and given any $x \in X$ we write $f(x) \in Y$ for the unique element satisfying $(x, f(x)) \in f$.

For such a function and classes $A \subseteq X$, $B \subseteq Y$ we write $f[A] := \{f(a) \mid a \in A\}$ for the *image* of A and $f^{-1}[B] := \{x \in X \mid f(x) \in B\}$ for the *preimage* of B . These definitions yield in an obvious way the *image function* $f[\cdot]: \mathcal{P}X \rightarrow \mathcal{P}Y$ and the *preimage function* $f^{-1}[\cdot]: \mathcal{P}Y \rightarrow \mathcal{P}X$. The *restriction* of f to A is the function $f|_A := f \cap A \times Y$ and denoted by $f|_A: A \rightarrow Y$.

A *partial function* is a relation $f \subseteq X \times Y$ such that $(x, y) \in f$ and $(x, z) \in f$ imply $y = z$. In this case we write $f: X \rightarrow Y$. Certainly every function is a partial function and conversely every partial function f yields a function $f|_A: A \rightarrow Y$ by restricting f to the set $A := \{x \in X \mid \exists y \in Y. (x, y) \in f\}$.

The set of *natural numbers* (without 0) is denoted by \mathbb{N} and we write \mathbb{N}_0 for the set $\mathbb{N} \cup \{0\}$. For the set of *integers* we use the symbol \mathbb{Z} and for the set of *rational numbers* we use \mathbb{Q} . The set of *real numbers* is denoted by \mathbb{R} and by adding the symbols ∞ (infinity) and $-\infty$ (minus infinity) together with the requirement $-\infty < r < \infty$ for all $r \in \mathbb{R}$ we obtain the set of extended reals $\overline{\mathbb{R}} := \mathbb{R} \cup \{\pm\infty\}$. The sets \mathbb{R}_+ and $\overline{\mathbb{R}}_+$ are their restrictions to the non-negative subsets. Apart from obvious choices for addition involving $\pm\infty$, we require $0 \cdot \pm\infty = \pm\infty \cdot 0 = 0$. For $a, b \in \overline{\mathbb{R}}$ we define the *open interval* $]a, b[:= \{r \in \overline{\mathbb{R}} \mid a < r < b\}$, the *closed interval* $[a, b] := \{r \in \overline{\mathbb{R}} \mid a \leq r \leq b\}$ and the *half open intervals* $]a, b] := \{r \in \overline{\mathbb{R}} \mid a < r \leq b\}$ and $[a, b[:= \{r \in \overline{\mathbb{R}} \mid a \leq r < b\}$.

If $Y \subseteq \overline{\mathbb{R}}$ and $f, g: X \rightarrow Y$ are functions we write $f \leq g$ if $\forall x \in X : f(x) \leq g(x)$. Moreover, the *support* of f is the set $\text{supp}(f) := \{x \in X \mid f(x) \neq 0\}$.

A *subprobability distribution* on a given set X is a function $P: X \rightarrow [0, 1]$ satisfying $\sum_{x \in X} P(x) \leq 1$ where for infinite X , the sum $\sum_{x \in X} P(x)$ is defined as the supremum $\sup \{ \sum_{x \in X'} P(x) \mid X' \subseteq X \wedge |X'| < \infty \}$. Using this we moreover define, for any set $B \subseteq X$, $P(B) = \sum_{x \in B} P(x)$. If $P(X) = 1$ we call P a *probability distribution*.

We will sometimes employ λ -*abstraction* in order to define functions. If T is a term with free variable x , we will write $\lambda x.T$ to denote an “assignment rule” from elements of a set $x' \in X$ to a term $T[x']$ where every occurrence of x is replaced with the element x' of X . In contrast to the usual definition in λ -calculus we implicitly assume some typing of all these terms $T[x']$ in such a way that they are elements of another set Y . Thus, for us $\lambda x.T$ denotes the function $f: X \rightarrow Y$ where $f(x) = T[x]$.

2.1.3 Ordinals and Transfinite Induction

A well-known proof technique for statements about natural numbers is the principle of *induction*. We will recall the basic ideas and then briefly explain a generalization of this technique called *transfinite induction*, which we will use in Chapters 4 and 5. For a more detailed, formal account of this, the reader is referred e.g. to Paul Bernay’s *System of Axiomatic Set Theory, Part II* [Ber41].

Let us suppose we are given a unary predicate Φ on a set X containing the natural numbers (i.e., $\mathbb{N}_0 \subseteq X$) which we can represent as a function $\Phi: X \rightarrow 2$. For any $x \in X$ we say that the predicate is *true* if $\Phi(x) = 1$ and it is *false* if $\Phi(x) = 0$. In order to show that Φ is true on every natural number, it suffices to carry out two steps: As first step we prove that $P(0) = 1$ holds (this is called the *base case*). Then we show that if $P(n) = 1$ holds for a natural number $n \in \mathbb{N}_0$ (this hypothesis is called the *induction hypothesis*) also $P(n+1)$ holds (this implication is called the *inductive step*).

In order to generalize this, we first observe that the natural numbers can be defined in set theory as follows.

$$\begin{aligned} 0 &:= \emptyset, \\ 1 &:= \{\emptyset\} \\ 2 &:= \{\emptyset, \{\emptyset\}\} \\ 3 &:= \{\emptyset, \{\emptyset\}, \{\emptyset, \{\emptyset\}\}\} \\ &\vdots \\ n+1 &:= n \cup \{n\} \end{aligned}$$

With this inductive definition, which is due to John von Neumann [vNeu23], we can see that each natural number n is the union of all its predecessors, i.e.,

$$n = \bigcup_{m \subseteq n} m.$$

Using the axioms of our suitably rich set theory we can deduce that there is a smallest set which contains all the natural numbers as defined above. This is the set \mathbb{N}_0 of all natural numbers which we also denote by ω in this context. It satisfies

$$\omega = \bigcup_{n \subseteq \omega} n.$$

Using these observations as intuition, we can now proceed to give a definition of the so-called *ordinals*, using the notation $0 := \emptyset$ and $\alpha + 1 := \alpha \cup \{\alpha\}$ for any set α .

Definition 2.1.1 (Ordinal, [Ber41, p. 10]) A set α is an *ordinal* if

1. either $0 = \alpha$ or $0 \in \alpha$, and
2. if $a \in \alpha$ then $a + 1 = \alpha$ or $a + 1 \in \alpha$, and
3. if $A \subseteq \alpha$ then $\bigcup A = \alpha$ or there is an $a \in \alpha$ such that $\bigcup A = a$.

We call an ordinal β a *successor (ordinal)* if there is an ordinal α such that $\beta = \alpha + 1$ and in this context we call α a *predecessor* of β . An ordinal γ without predecessors is called a *limit (ordinal)*. Clearly it satisfies $\gamma = \bigcup_{\alpha < \gamma} \alpha$.

Using this terminology, we can easily see that both 0 and ω are limit ordinals whereas any natural number $n > 0$ is a successor ordinal. Moreover, we can define new ordinals like $\omega + 1$, $\omega + 2 := (\omega + 1) + 1$ and so on, as well as $\omega + \omega = \omega \cdot 2 = \bigcup_{n \in \omega} (\omega + n)$. All ordinals considered so far are countable sets: the natural numbers are finite sets and all the other ordinals α , starting with ω , are countably infinite, i.e., there exists a bijective function $f: \omega \rightarrow \alpha$. The union of all countably infinite ordinals is again an ordinal, the first uncountable ordinal ω_1 . By definition each ordinal is a set but it can be shown that the class of all ordinals, denoted as Ord , is not a set.

If we want to prove a statement about ordinal numbers, we can use *transfinite induction*. Suppose we are given a predicate Φ on a class X including ordinal numbers, i.e., a function $\Phi: X \rightarrow 2$ with $\text{Ord} \subseteq X$. If we can prove that

1. $\Phi(0)$ is true, and
2. if $\Phi(\alpha)$ is true for an ordinal α , then so is $\Phi(\alpha + 1)$, and

3. if β is a limit ordinal and $\Phi(\alpha)$ is true for all ordinals $\alpha < \beta$ then so is $\Phi(\beta)$
 we may conclude that $\Phi(\alpha) = 1$ holds for all ordinals $\alpha \in \text{Ord}$.

2.2 Transition Systems and Automata

We assume that the reader is familiar with labelled transition systems and in particular with automata theory. However, for reasons of clarity and to introduce our notation we recall a few basics here. For more detailed information we suggest e.g. the extensive textbook *Principles of Model Checking* by Christel Baier and Joost-Pieter Katoen [BKo8].

2.2.1 Labelled Transition Systems

First of all, let us recall the essential definitions of (labelled) transition systems and some notational conventions.

Definition 2.2.1 (Transition System, Labelled Transition System) A *transition system* is a pair (X, \rightarrow) consisting of a set X of *states* and a binary relation $\rightarrow \subseteq X \times X$ called the *transition relation* which is usually written in infix notation, i.e., instead of $(x, y) \in \rightarrow$ we write $x \rightarrow y$ and we call y a *successor* (state) of x . We write $x \nrightarrow$ if there is no $y \in X$ such that $x \rightarrow y$.

Similarly, a *labelled transition system* (LTS) is a triple (X, A, \rightarrow) , consisting of a set X of *states*, a (usually finite) set A of *actions* or *transition labels* and a ternary relation $\rightarrow \subseteq X \times A \times X$ called the *transition relation*. As above, instead of $(x, a, y) \in \rightarrow$ we write $x \xrightarrow{a} y$ and we call y an *a-successor* of x . Moreover, we write $x \xrightarrow{a}$ if there is no $y \in X$ such that $x \xrightarrow{a} y$ and finally $x \nrightarrow^a$ if there is no $a \in A$ such that $x \xrightarrow{a}$.

Our main interest in this thesis are labelled transition systems since our aim is to compare behavior which is based on the labels which can be either interpreted as *input* or *output* (we will discuss this in Section 2.2). In order to work with labels, we need to talk about words and the free monoid construction.

Words and the Free Monoid Construction

We recall that for any set A (not necessarily finite) the set A^* consists of all finite-length (possibly zero) strings of elements of A , called *words*. Explicitly, let ε be a fresh (i.e. $\varepsilon \notin A$) symbol which is called the *empty word* (its length is zero). We now define $A_0 := \{\varepsilon\}$, $A_1 := A$, $A_{n+1} := \{wa \mid w \in A_n, a \in A\}$ for $n \in \mathbb{N}$ which are the sets of finite words of length n . Then A^* is the union of

all these sets, i.e., $A^* := \bigcup_{n \in \mathbb{N}_0} A_n$. Since the elements of A^* are called words, we usually call the elements of A *letters* and A itself an *alphabet*¹.

Given two words $v, w \in A^*$ we can *concatenate* them simply by appending all the letters of w to v , i.e., we obtain the new word $vw \in A^*$. This yields a function $\cdot : A^* \times A^* \rightarrow A^*$ which we always write in infix notation (and usually, we will even omit the dot). It is *associative*, i.e., $(u \cdot v) \cdot w = u \cdot (v \cdot w)$ holds for all $u, v, w \in A^*$ and the empty word serves as a both-sided *neutral element*, i.e., $u \cdot \varepsilon = \varepsilon \cdot u = u$. Thus A^* together with the concatenation is a *monoid*, the so-called *free monoid* on A .

We denote the length of a word $w \in A^*$ as $|w| \in \mathbb{N}_0$. It will sometimes be convenient to consider words up to a predefined length $n \in \mathbb{N}_0$, i.e., we will consider the sets $A^{\leq n} := \bigcup_{i=0}^n A_i = \{w \in A^* \mid |w| \leq n\}$.

An *infinite word* is a function $v : \mathbb{N}_0 \rightarrow A$ and the set of all these words is traditionally denoted² by A^ω . The set of all finite and infinite words is the set $A^\infty := A^* \cup A^\omega$. We can obviously concatenate a finite word $w \in A^*$ and an infinite one $v \in A^\omega$ to obtain the infinite word $wv = w \cdot v \in A^\omega$ but it is impossible to append w to v .

Having these definitions at hand, we can now extend the transition relation of a labelled transition system to arbitrary words. First we extend $\rightarrow \subseteq X \times A \times X$ to a relation $\rightarrow^* \subseteq X \times A^* \times X$. Certainly we want $\rightarrow \subseteq \rightarrow^*$. Moreover, for every state $x \in X$ we define $(x, \varepsilon, x) \in \rightarrow^*$. For states $x, y \in X$ and a word $w = a_0 \dots a_n \in A^*$ of length $n + 1$ with $n \geq 1$ we define $x \xrightarrow{w}^* y$ if there are states $x_0, \dots, x_{n+1} \in X$ such that $x = x_0$, $y = x_{n+1}$ and $x_i \xrightarrow{a_i} x_{i+1}$ for every $i \in \{0, \dots, n\}$. Naturally we write $x \xrightarrow{w}$ if there is no $y \in X$ such that $x \xrightarrow{w}^* y$. Finally, for infinite words $w \in A^\omega$ we write $x \xrightarrow{w}^\omega$ if there exists a function $r : \mathbb{N}_0 \rightarrow X$ mapping natural numbers to states such that $r(0) = x$ and for all $n \in \mathbb{N}_0$ we have a transition $x_n \xrightarrow{w(n)} x_{n+1}$. If such a function does not exist, we also write $x \not\xrightarrow{w}^\omega$.

2.2.2 Trace Equivalence and Bisimulation

The two most prominent notions of behavior for labelled transition systems are trace equivalence and bisimulation. The conceptually very simple notion of *language* or *trace equivalence* will later turn out to be more difficult to handle coalgebraically than the more complicated notion of *bisimilarity*. Let us quickly recap their formal definitions.

¹Later we will often require an alphabet to be at least countable or even finite.

²Of course, it is also legitimate to denote them by $A^{\mathbb{N}_0}$.

Definition 2.2.2 (Language/Trace of a State) Let (X, A, \rightarrow) be an LTS. For every state $x \in X$ we define the sets

$$\mathcal{L}^*(x) := \{w \in A^* \mid x \xrightarrow{w}^*\} \subseteq A^*, \quad (2.2.1)$$

$$\mathcal{L}^\omega(x) := \{w \in A^\omega \mid x \xrightarrow{w}^\omega\} \subseteq A^\omega, \quad (2.2.2)$$

$$\mathcal{L}^\infty(x) := \mathcal{L}^*(x) \cup \mathcal{L}^\omega(x) \subseteq A^\infty, \quad (2.2.3)$$

which are called the the finite/infinite *languages* or *traces* of x . Two states $x, y \in X$ are called *language equivalent* or *trace equivalent* whenever $\mathcal{L}^*(x) = \mathcal{L}^*(y)$ (and analogously for the other two cases).

The traces induce relations $R \subseteq X \times X$ on the set of states, e.g. for \mathcal{L}^* we define $xRy : \iff \mathcal{L}^*(x) = \mathcal{L}^*(y)$. It is easy to see that such a relation is indeed an *equivalence relation*, i.e., it is *reflexive* (xRx holds for all $x \in X$), *symmetric* ($xRy \implies yRx$) and *transitive* ($xRy \wedge yRz \implies xRz$), which justifies the name *trace equivalence*.

Before continuing, let us illustrate traces with a standard example.

Example 2.2.3 We consider the labelled transition system depicted in Figure 2.2.1 with state space $X = \{x_1, x_2, x_3, x_4, x_5, y_1, y_2, y_3, y_4\}$ and alphabet $A = \{a, b, c\}$. Obviously there are no infinite paths in these systems, so we just

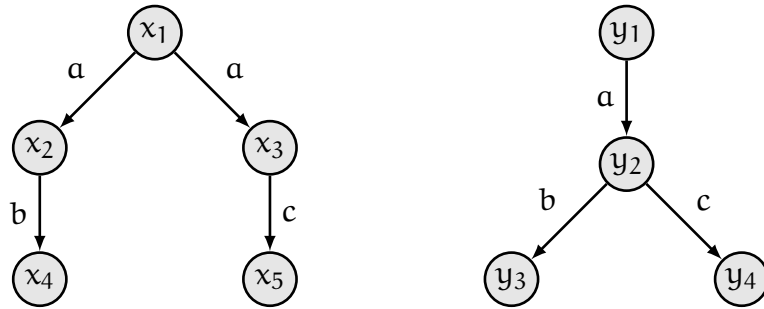


Figure 2.2.1: A labelled transition system

consider finite traces where we have $\mathcal{L}^*(x_4) = \mathcal{L}^*(x_5) = \mathcal{L}^*(y_3) = \mathcal{L}^*(y_4) = \{\varepsilon\}$, $\mathcal{L}^*(x_2) = \{\varepsilon, b\}$, $\mathcal{L}^*(x_3) = \{\varepsilon, c\}$, $\mathcal{L}^*(y_2) = \{\varepsilon, b, c\}$, and $\mathcal{L}^*(x_1) = \{\varepsilon, a, ab, ac\} = \mathcal{L}^*(y_1)$. Thus x_1 and y_1 are *trace equivalent*.

Although the states x_1 and y_1 in the above example are trace equivalent, there is an apparent difference between them. Suppose we wanted to do a two step transition from either of them, then for sure the first action will have to be an a . However, for x_1 it is important to take the correct transition which depends

on the second action (if it is a b we need to take the left branch, otherwise the right one). For y_1 this decision is delayed to the second action. This branching difference can be captured by a finer equivalence relation on the state space, the bisimilarity.

Definition 2.2.4 (Bisimulation, Bisimilar, Bisimilarity) Let (X, A, \rightarrow) be a labelled transition system

1. A binary relation $R \subseteq X \times X$ is called a *bisimulation* if it satisfies the following requirements for every pair $(x, y) \in R$ and every action $a \in A$.
 - ▷ For every $x' \in X$ with $x \xrightarrow{a} x'$ there is a $y' \in X$ such that $y \xrightarrow{a} y'$ and $(x', y') \in R$.
 - ▷ For every $y' \in X$ with $y \xrightarrow{a} y'$ there is an $x' \in X$ such that $x \xrightarrow{a} x'$ and $(x', y') \in R$.
2. Two states $x, y \in Y$ are *bisimilar* (denoted by $x \sim y$) if there is a bisimulation R such that $(x, y) \in R$. The resulting relation \sim is called *bisimilarity*.

Let us look at the LTS of Example 2.2.3 again and convince ourselves that states x_1 and y_1 are *not bisimilar*. Let us assume they were, i.e., we assume that there was a bisimulation relation $R \subseteq X \times X$ such that $(x_1, y_1) \in R$. Then, by the definition of bisimulation, we would also need $(x_2, y_2) \in R$ but this is impossible since from y_2 we have a c -transition (to y_4) but there is no c -transition from x_2 . Thus our assumption was false and x_1 and y_2 are indeed not bisimilar.

There are a few more remarks in order. First of all, a bisimulation is not necessarily an equivalence. If we again consider the transition system of Example 2.2.3, it is easy to check that $\{(x_4, x_5), (x_5, y_3)\}$ is a bisimulation which is neither reflexive, nor symmetric, nor transitive. However, we can quickly convince ourselves that the identity relation $\text{id}_X := \{(x, x) \mid x \in X\}$ is a bisimulation and for any bisimulation R also its inverse $R^{-1} := \{(x, y) \mid (y, x) \in R\}$ is a bisimulation. Moreover, given two bisimulations R_1, R_2 also their composition $R_1 R_2$ and their (set theoretic) union is again a bisimulation. Based on these observations it is easy to conclude that the bisimilarity is an equivalence relation and additionally that it is also the largest bisimulation with respect to set inclusion. For finite transition systems the bisimilarity can thus be computed using partition refinement starting with the largest equivalence relation $\sim_0 = X \times X$.

As a last remark we recall that bisimilarity is *finer* than trace equivalence in the sense that if x and y are bisimilar they are also trace equivalent but the converse is not necessarily true as the above transition systems show. However, for deterministic systems language and trace equivalence can be shown to coincide.

2.2.3 Side Effects: From Nondeterminism To Probability

If we interpret the labels of the transitions as *input* to which the system reacts, it is more intuitive to rewrite the transition relation \rightarrow as a function $\delta: X \times A \rightarrow \mathcal{P}X$. Thus for each state $x \in X$ and each input $a \in A$ the set $\delta(x, a) \subseteq X$ describes the set of a -successors of x . The system reacts to the given input by choosing nondeterministically a state $y \in \delta(x, a)$ and then moves to that state. Now if we assume that both X and A are finite sets, specify a subset $I \subseteq X$ of *initial states* and another subset $F \subseteq X$ of final states we recover the classical definition of a *nondeterministic finite automaton* (NFA) which is then written as quintuple $\mathcal{A} = (X, A, \delta, I, F)$.

If we require for an LTS that for each action $a \in A$ there is always a unique a -successor, we can write the transition relation as function $\delta: X \times A \rightarrow X$. Thus, for each state $x \in X$ and each input $a \in A$ the system deterministically moves from x to the state $\delta(x, a) \in X$. By adding a distinct initial state $x_0 \in X$ and a set $F \subseteq X$ of final states and requiring finiteness of both X and A we recover the classical definition of a *deterministic finite automaton* (DFA) which then is written as quintuple $\mathcal{A} = (X, A, \delta, x_0, F)$.

For both deterministic and nondeterministic automata alike the final states have to be taken into account for the behavioral analysis. In contrast to arbitrary LTS, the language of a state $x \in X$ of an automaton is defined to be the set

$$\mathcal{L}(x) := \left\{ w \in A^* \mid \exists y \in F. x \xrightarrow{w}^* y \right\} \subseteq A^* \quad (2.2.4)$$

of all finite words $w \in A^*$ for which there exists a path from x to a *final* state $y \in Y$ in the underlying transition systems whose labels are the letters of w .

Similarly, for a bisimulation relation $R \subseteq X \times X$ on the state space of an automaton we need to add the requirement that xRy implies that either both states are final or both are non-final.

Note that the initial states do not play a significant role in the definition or comparison of behavior of states. They are only needed in order to talk about the behavior of the whole automaton, which is just defined to be the behavior of the initial state(s). This observation is important to understand the coalgebraic view in which we will usually not specify initial states.

Probabilistic Systems

Let us finish this section with another type of automata. As said before, in the case of a nondeterministic automaton we think of the system as reacting to a given input $a \in A$ by moving from its current state $x \in X$ to one of the states in the set $\delta(x, a)$. In this setting it can of course happen that there is no

α -transition from x if $\delta(x, \alpha) = \emptyset$ and thus the system simply cannot accept an α -input. However, a more interesting situation arises if there is more than one possible α -successor. Here it is important to understand that a nondeterministic choice does not model any information about the likelihood. We can neither assume that one α -successor is more likely than another nor should we think of them as being equally likely.

In order to make statements about this, we need to consider *probabilistic transition systems* where we replace the nondeterministic choice by a probabilistic one. Since there are many variants of these probabilistic system, let us make explicit which definitions we are going to use. The first type of system regards actions as inputs to which the system reacts [LS89, Definition 2.1].

Definition 2.2.5 (Reactive Probabilistic Transition System) A *reactive probabilistic transition system* is a triple (X, A, δ) where X is a set of states, A is a set of actions and $\delta: X \times A \rightarrow \mathcal{D}X$ is the probabilistic transition function mapping pairs of a state and an action to a subdistribution satisfying³ $\delta(x, a)(X) \in \{0, 1\}$.

If such a system is in a state $x \in X$ and reads an input action $a \in A$ it behaves as follows: if $\delta(x, a)(X) = 1$ the system chooses an a -successor according to the probability distribution $\delta(x, a): X \rightarrow [0, 1]$ and moves to that state. Otherwise, if $\delta(x, a)(X) = 0$ the system cannot accept the action a in that state.

Naturally, bisimulations for such systems need to take into account the probabilities. For a detailed discussion of this the reader is referred to Kim G. Larsen's and Arne Skou's papers [LS89; LS91] where probabilistic bisimulation was first introduced. This is also the reason why it is sometimes called *Larsen-Skou* bisimulation.

Definition 2.2.6 (Probabilistic Bisimulation [LS89, Definition 6.3]) An equivalence relation $R \subseteq X \times X$ on the state space of a reactive probabilistic transition system (X, A, δ) is called a *probabilistic bisimulation* if

$$\delta(x, a)(S) = \delta(x', a)(S)$$

holds for all $(x, x') \in R$, all $a \in A$ and all equivalence classes $S \in X/R$.

Two states $x, x' \in X$ are called *probabilistically bisimilar* if there is a probabilistic bisimulation R such that $(x, x') \in R$. The resulting relation is called *probabilistic bisimilarity*.

In contrast to ordinary bisimulations, the probabilistic variant only allows equivalence relations to be bisimulations.

³Recall that $\delta(x, a)$ is a subdistribution, thus $\delta(x, a)(X) = \sum_{x' \in X} \delta(x, a)(x')$.

As explained above, the reactive probabilistic transition systems, also known as *Markov decision processes (MDP)* (without rewards), react to an input $a \in A$ which has to be provided by a user or the environment. Thus we have no information about the likelihood of the labels. If we want to have that as well, we can consider systems whose transitions are slightly different. We will discuss such systems in detail in Chapter 4 (but also confer to the referenced literature by Ana Sokolova and Erik P. de Vink [SdVo4; Sok05; Sok11] for an overview of these and various other probabilistic systems).

Definition 2.2.7 (Generative Probabilistic Transition System) A *generative probabilistic transition system* is a triple (X, A, δ) , where X is a set of states, A is a set of actions and $\delta: X \rightarrow \mathcal{D}(A \times X + \mathbb{1})$ is the transition function mapping each state to a subprobability distribution on⁴ $A \times X + \mathbb{1}$.

For each state $x \in X$ the function $\delta(x): A \times X + \mathbb{1} \rightarrow [0, 1]$ describes the probability of termination ($\delta(x)(\checkmark)$) and for each pair (a, y) of a label $a \in A$ and a state $y \in X$ the probability of moving from state x to y while outputting an a . The sum $\sum_{y \in X} \delta(x)(a, y)$ describes the total probability of traversing an a -transition from x to another state, whereas the sum $\sum_{a \in A} \delta(x)(a, y)$ describes the probability of traversing a transition from x to a fixed state $y \in Y$, irrespective of the transition label. Since for these systems all the information about the transitions is given, they are called *generative* probabilistic transition systems. From any given state, they probabilistically generate a sequence of labels so it makes sense to think of the labels as an *output* of the system. As for conventional labelled transition systems we can consider the traces of these systems which are words in A^* . Using the probabilistic information we have, we can not only say which words are generated but also with what probability they are generated.

Definition 2.2.8 (Probabilistic Trace) The *trace* of a state $x \in X$ of a generative probabilistic system (X, A, δ) is the probability distribution $\text{tr}(x): A^* \rightarrow [0, 1]$ given by

$$\text{tr}(x)(\varepsilon) = \delta(x)(\varepsilon), \quad (2.2.5)$$

$$\forall a \in A. \forall w \in A^*. \text{tr}(x)(aw) = \sum_{y \in X} \text{tr}(y)(w) \cdot \delta(x)(a, y) \quad (2.2.6)$$

which assigns to each word $w \in A^*$ the probability of being generated by the given probabilistic transition system.

As final remark on probabilistic systems we note that the systems presented so

⁴Recall that $+$ denotes the disjoint union of sets and $\mathbb{1} = \{\checkmark\}$.

far are *discrete systems*, i.e., their probabilistic branching is limited to a countable set: We recall that for infinite sets X and a function $P: X \rightarrow [0, 1]$ we defined the sum as

$$P(X) = \sum_{x \in X} P(x) := \sup \left\{ \sum_{x \in X'} P(x) \mid X' \subseteq X \text{ and } X' \text{ is finite} \right\}.$$

It can be shown [Sok11] that the requirement $P(X) \leq 1$ automatically implies that the support of P , i.e., the set $\{x \in X \mid P(x) > 0\}$ is countable. In order to model arbitrary probabilistic system it is necessary to move to a much more general, measure theoretic setting where it is possible to use integration. We will take this route in Chapter 4 and use it to consider not only arbitrary infinite systems but also *infinite traces* for probabilistic systems which cannot be captured in the discrete setting.

2.3 Category Theory

Category theory is an abstract mathematical framework which tries to identify the crucial properties of mathematical objects and get rid of specific details. It can thus be understood as an attempt to unify the languages of different areas of mathematics.

Note that this section has no immediate apparent connection to the previous one but we will establish a connection when we discuss coalgebra in the succeeding section. Moreover, this section does not (and is not meant to) provide a complete introduction to this highly complex topic. We will just provide the definitions and results needed later in this thesis, accompanied by some very brief explanations. Therefore this section serves two purposes: It makes the thesis self-contained so there is no (immediate) need to consult other literature and it fixes the notation we will use in the later parts.

In order to learn more about category theory, the interested reader is invited to look into Saunders Mac Lane's classical *Categories for the Working Mathematician* [Mac98], the freely available *Abstract and Concrete Categories – The Joy of Cats* by Jiří Adámek, Horst Herrlich and George E. Strecker [AHS90] or *Category Theory* [Awo06] by Steve Awodey to mention just a few.

2.3.1 Basics

Frequently, mathematical objects arise together with a notion of morphism between them that respects the properties of these objects. For example, one considers sets and functions, groups and group homomorphisms or vector

spaces and linear maps just to mention a few of them. In the most basic definition of category theory – a category – we axiomatically state the essential laws such a combination of objects and morphisms should satisfy.

In the literature there are several distinct but equivalent definitions. We will start with the following definition and later briefly discuss some alternatives.

Definition 2.3.1 (Category) A category \mathfrak{C} consists of

- ▷ a class \mathcal{O} whose elements are called *objects*,
- ▷ a class $\mathfrak{C}(A, B)$ for all objects $A, B \in \mathcal{O}$ whose elements are called *arrows* or *morphisms*,
- ▷ an *identity arrow* $\text{id}_A \in \mathfrak{C}(A, A)$ for each object $A \in \mathcal{O}$, and
- ▷ a *composition function* $\circ: \mathfrak{C}(B, C) \times \mathfrak{C}(A, B) \rightarrow \mathfrak{C}(A, C)$ for all objects $A, B, C \in \mathcal{O}$ which assigns to any arrow $f \in \mathfrak{C}(A, B)$ and $g \in \mathfrak{C}(B, C)$ their *composite* $gf := g \circ f$

such that

1. the classes of arrows are disjoint, i.e. for all objects $A, B, C, D \in \mathcal{O}$ we require that if $(A, B) \neq (C, D)$, then $\mathfrak{C}(A, B) \cap \mathfrak{C}(C, D) = \emptyset$,
2. composition is associative, i.e. for all objects $A, B, C, D \in \mathcal{O}$ and all arrows $f \in \mathfrak{C}(A, B)$, $g \in \mathfrak{C}(B, C)$, $h \in \mathfrak{C}(C, D)$ we require $h \circ (g \circ f) = (h \circ g) \circ f$, and
3. the identities are neutral wrt. to the composition, i.e. for all objects $A, B \in \mathcal{O}$ and all arrows $f \in \mathfrak{C}(A, B)$ we require $f \circ \text{id}_A = f = \text{id}_B \circ f$.

In order to differentiate the object classes of different categories, we will sometimes use the notation $\mathcal{O}(\mathfrak{C})$ or – by abuse of notation – frequently write $A \in \mathfrak{C}$ for $A \in \mathcal{O}(\mathfrak{C})$.

The class of all arrows of \mathfrak{C} is the union $\mathbb{A} := \cup_{A, B \in \mathcal{O}} \mathfrak{C}(A, B)$. By Axiom 1 for each element $f \in \mathbb{A}$ there is a unique pair $(A, B) \in \mathcal{O} \times \mathcal{O}$ such that $f \in \mathfrak{C}(A, B)$. We call A the *source* or *domain* of f and denote it by $\text{dom}(f)$ and B the *target* or *codomain* of f and denote it by $\text{cod}(f)$. As above we write $\mathbb{A}(\mathfrak{C})$ if we want to emphasize the category to which the arrows belong.

Note that Axiom 1 imposes no real restriction for if the classes of arrows were not disjoint, we could simply define $\mathfrak{C}'(A, B) := \{A\} \times \mathfrak{C}(A, B) \times \{B\}$ and identify each $f \in \mathfrak{C}(A, B)$ bijectively with $(A, f, B) \in \mathfrak{C}'(A, B)$. The axiom is nevertheless useful since when we consider the class \mathbb{A} of all arrows we have a unique domain and codomain for each of its elements.

An alternative (but equivalent) way to define a category is to give the class of objects \mathcal{O} and the class of *all* morphisms \mathcal{A} together with two functions $\text{dom}, \text{cod}: \mathcal{A} \rightarrow \mathcal{O}$, a partial composition function $\circ: \mathcal{A} \times \mathcal{A} \rightarrow \mathcal{A}$ which has to be defined on exactly those pairs $(g, f) \in \mathcal{A} \times \mathcal{A}$ where $\text{dom}(g) = \text{cod}(f)$, and an identity arrow $\text{id}_A \in \mathcal{A}$ with $\text{dom}(\text{id}_A) = \text{cod}(\text{id}_A) = A$ for each objects \mathcal{O} satisfying (obvious) equivalents to Axioms 2 and 3. Then one simply defines, for all objects A, B the classes $\mathcal{C}(A, B) := \{f \in \mathcal{A} \mid \text{dom}(f) = A \wedge \text{cod}(f) = B\}$. For a more detailed discussion on this we refer to the first chapter of *Categories for the Working Mathematician* [Mac98]. We will freely switch between both definitions.

With a standard argument we can see that Axiom 3 implies that for each object A there is a *unique* identity arrow id_A . Indeed, for identity arrows $\text{id}_A, \text{id}'_A \in \mathcal{C}(A, A)$ the axiom tells us that $\text{id}'_A = \text{id}'_A \circ \text{id}_A = \text{id}_A$. Thus we can safely talk about *the* identity arrow of an object A and moreover, using this bijective correspondence one can yet give another, “arrows only”-definition of a category. Again we refer the reader to the text books given above for details.

Before we continue, we consider a few standard examples of categories which we will use later. The smallest category is the empty category with no objects and no morphisms. Other simple examples are given by $(\circ \rightarrow \circ \leftarrow \circ)$ or $(\circ \leftarrow \circ \rightarrow \circ)$ which are categories with three objects and (apart from the necessary identities) arrows as indicated by the graphical notation. The next example is our first example of a category with infinitely many objects and infinitely many arrows.

Example 2.3.2 (Category of Sets and Functions) The category *Set* has as objects the class of all sets and for all sets A, B the class $\text{Set}(A, B)$ consists of all functions $f: A \rightarrow B$. The identity arrow on a set A is the identity function $\text{id}_A: A \rightarrow A, a \mapsto a$ and the composition of arrows is function composition.

This simple example shows the need for classes: The class of all sets is a proper class and not a set. Certainly, this implies that also the class \mathcal{A} of all arrows of this category is a proper class. However, one can prove that each class $\text{Set}(A, B)$ of functions from a set A to a set B is itself a set which we will also denote by B^A . We will take these observations as a motivation for the following definition.

Definition 2.3.3 (Large, Small, Locally Small, Discrete) We call a category \mathcal{C}

1. *large* if \mathcal{O} is a proper class,
2. *small* if \mathcal{O} is a set,
3. *locally small* if for all $A, B \in \mathcal{O}$ the class $\mathcal{C}(A, B)$ is a set, or

4. *discrete* if for all $A, B \in \mathcal{O}$ we have $\mathcal{C}(A, B) = \{\text{id}_A\}$ if $A = B$ and $\mathcal{C}(A, B) = \emptyset$ if $A \neq B$.

In this terminology, *Set* is a large and locally small category (but certainly not discrete). Many of the categories in this thesis will be of this type. Let us consider another example.

Example 2.3.4 (Category of Monoids and Monoid Homomorphisms) Recall that a *monoid* is a triple (M, \circ, e) where

1. M is a set,
2. $\circ: M \times M \rightarrow M$ is an associative operation, i.e., for all $m_1, m_2, m_3 \in M$ we require $(m_1 \circ m_2) \circ m_3 = m_1 \circ (m_2 \circ m_3)$, and
3. $e \in M$ is a *neutral element* such that for all $m \in M$ we have $m \circ e = e \circ m = m$.

A *monoid homomorphism* between two monoids (M, \circ, e_M) and $(N, *, e_N)$ is a function $h: M \rightarrow N$ such that $h(e_M) = e_N$ and for all $m_1, m_2 \in M$ we have $h(m_1 \circ m_2) = h(m_1) * h(m_2)$. The monoids and the monoid homomorphism form a category which we denote by *Mon*.

It is imperative to understand that – although this is true for many of our examples – arrows are not necessarily “functions with structure”. A prototypical example where this is not the case, is the following.

Example 2.3.5 (Category of Sets and Relations) The category *Rel* has as objects all sets and for all sets A, B the class $\text{Rel}(A, B)$ consists of all relations, i.e. all subsets $R \subseteq A \times B$. The identity arrow on a set A is the identity relation $\text{id}_A = \{(a, a) \mid a \in A\}$ and given two relations $R \in \text{Rel}(A, B)$ and $S \in \text{Rel}(B, C)$ their composition is the relation $S \circ R := \{(a, c) \mid \exists b \in B. (a, b) \in R \wedge (b, c) \in S\}$ which is usually denoted in reverse order and without the circle, i.e., as RS .

The focus of category theory is on the arrows, not on the objects of categories. A crucial property of an arrow is invertibility as it shows when two objects are almost identical.

Definition 2.3.6 (Isomorphism, Isomorphic) Let \mathcal{C} be a category and $A, B \in \mathcal{O}$. We call an arrow $f \in \mathcal{C}(A, B)$ an *isomorphism* or short an *iso* if it is *invertible*, i.e. if there is an arrow $g \in \mathcal{C}(B, A)$ such that $f \circ g = \text{id}_B$ and $g \circ f = \text{id}_A$. We call A and B *isomorphic* if there is an isomorphism $f \in \mathcal{C}(A, B)$.

A similar (simple) argument as the one used above to show uniqueness of the identity arrows also proves uniqueness of the arrow g . Thus we can safely call

g the *inverse* to f and denote it by f^{-1} . Isomorphisms play an important role in many category theoretic definitions, because these definitions specify objects (along with arrows) up to isomorphism. We will discuss this issue further in Section 2.3.3. Here we just mention that in \mathbf{Set} the isomorphisms are exactly the bijective functions.

We can also give a categorical generalization of surjective and injective functions, so-called epi- and monomorphisms.

Definition 2.3.7 (Epimorphism, Monomorphism) Let \mathcal{C} be a category and $A, B \in \mathcal{O}$ be objects. We call an arrow $f \in \mathcal{C}(A, B)$

1. an *epimorphism*, short *epi*, if it is *right-cancellative*, i.e., if for any two arrows $g_1, g_2 \in \mathcal{C}(B, C)$ the equality $g_1 \circ f = g_2 \circ f$ implies $g_1 = g_2$.
2. a *monomorphism*, short *mono*, if it is *left-cancellative*, i.e., if for any two arrows $g_1, g_2 \in \mathcal{C}(C, A)$ the equality $f \circ g_1 = f \circ g_2$ implies $g_1 = g_2$.

It is easy to see that every isomorphism is both an epimorphism and a monomorphism. Moreover, if an arrow $f \in \mathcal{C}(A, B)$ has a right inverse, i.e., a function $g \in \mathcal{C}(B, A)$ such that $fg = \text{id}_B$, this arrow is an epi. In this case we call f a *split epi* and similarly we call it a *split mono* if it has a left inverse.

For any category we can construct another category by simply turning the arrows around.

Definition 2.3.8 (Dual Category, Opposite Category) Let \mathcal{C} be a category. The *dual category* (or *opposite category*), denoted \mathcal{C}^{op} , has the same objects and identities as \mathcal{C} and for all $A, B \in \mathcal{O}$ we define $\mathcal{C}^{\text{op}}(A, B) := \mathcal{C}(B, A)$. Given arrows $f \in \mathcal{C}^{\text{op}}(A, B)$, $g \in \mathcal{C}^{\text{op}}(B, C)$, their composition is defined by taking the corresponding arrows $f' \in \mathcal{C}(B, A)$, $g' \in \mathcal{C}(C, B)$, composing them in \mathcal{C} to the arrow $h' := f' \circ g' \in \mathcal{C}(C, A)$ and then taking the corresponding arrow $h \in \mathcal{C}^{\text{op}}(A, C)$ as the composite $g \circ f$.

The arrows of \mathbf{Set}^{op} are thus relations whose inverses are functions. Since the inverse of a relation is also a relation, \mathbf{Rel} is a so-called *self-dual* category, i.e., \mathbf{Rel}^{op} is “essentially the same” as \mathbf{Rel} . We will later (in Section 2.3.4) see how this can be made precise.

Another way to construct a new category out of given ones is described in the next definition. Apparently this definition can be extended to finitely many categories.

Definition 2.3.9 (Product Category) Let \mathcal{C}, \mathcal{D} be categories. The *product category* of \mathcal{C} and \mathcal{D} , denoted $\mathcal{C} \times \mathcal{D}$, has as objects the class of all pairs (X, Y) of objects

$X \in \mathfrak{C}$, $Y \in \mathfrak{D}$ and as arrows all pairs (f, g) of arrows $f \in \mathbb{A}(\mathfrak{C})$, $g \in \mathbb{A}(\mathfrak{D})$. The identities are all the pairs of identity arrows and composition of arrows is done componentwise, i.e., $(f, g) \circ (h, k) = (f \circ h, g \circ k)$.

2.3.2 Functors

Besides considering the arrows within a category, it is also natural to consider arrows between categories, so-called *functors*.

Definition 2.3.10 (Functor) Let \mathfrak{C} and \mathfrak{D} be categories. A (covariant) *functor* from \mathfrak{C} to \mathfrak{D} , denoted by $F: \mathfrak{C} \rightarrow \mathfrak{D}$, consists of a function $F_0: \mathcal{O}(\mathfrak{C}) \rightarrow \mathcal{O}(\mathfrak{D})$ and functions $F_{A,B}: \mathfrak{C}(A, B) \rightarrow \mathfrak{D}(F_0A, F_0B)$ for all objects $A, B \in \mathcal{O}(\mathfrak{C})$ such that

1. identities are preserved, i.e., for all objects $A \in \mathcal{O}(\mathfrak{C})$ we require that $F_{A,A}(\text{id}_A) = \text{id}_{F_0A}$, and
2. composition is preserved, i.e., for all objects $A, B, C \in \mathcal{O}(\mathfrak{C})$ and all arrow $f \in \mathfrak{C}(A, B)$, $g \in \mathfrak{C}(B, C)$ we require $F_{B,C}(g) \circ F_{A,B}(f) = F_{A,C}(g \circ f)$.

To simplify the notation we will write FA for F_0A and Ff instead of $F_{A,B}f$. If $\mathfrak{C} = \mathfrak{D}$ we call F an *endofunctor* on \mathfrak{C} .

There are two obvious examples of functors. The first is an endofunctor, the *identity functor* $\text{Id}_{\mathfrak{C}}: \mathfrak{C} \rightarrow \mathfrak{C}$, also written as $_ : \mathfrak{C} \rightarrow \mathfrak{C}$ which maps every object to itself and every arrow to itself. Given an object $D \in \mathcal{O}(\mathfrak{D})$ the *constant D-functor* is the functor $F: \mathfrak{C} \rightarrow \mathfrak{D}$ defined as $FA = D$ for every object $A \in \mathcal{O}$ and $Ff = \text{id}_D$ for every $f \in \mathbb{A}(\mathfrak{C})$. A more interesting example is the powerset functor.

Example 2.3.11 (Powerset Functors) The *powerset functor* $\mathcal{P}: \text{Set} \rightarrow \text{Set}$ maps each set A to its powerset $\mathcal{P}A := \{S \mid S \subseteq A\}$ and every function $f: A \rightarrow B$ to the image function $f[\cdot]: \mathcal{P}A \rightarrow \mathcal{P}B$, $f[S] := \{f(a) \mid a \in S\}$. The *finite powerset functor* $\mathcal{P}_f: \text{Set} \rightarrow \text{Set}$ maps each set A to the set of all its finite subsets, i.e. $\mathcal{P}_fA := \{S \mid S \subseteq A \wedge |S| < \infty\}$. On functions it is defined as the powerset functor.

We will encounter the powerset functor and its finite variant quite often in this thesis. The same is true for the (probability) distribution functor.

Example 2.3.12 (Distribution Functors) The *distribution functor* $\mathcal{D}: \text{Set} \rightarrow \text{Set}$ maps each set A to the set of all *probability distributions*, i.e., the set

$$\mathcal{D}A := \left\{ p: A \rightarrow [0, 1] \mid \sum_{a \in A} p(a) = 1 \right\}, \quad (2.3.1)$$

and every function $f: A \rightarrow B$ to the function $\mathcal{D}f$ which is defined, for all distributions $p \in \mathcal{D}A$ and all $b \in B$, via

$$\mathcal{D}f(p)(b) = \sum_{a \in f^{-1}[\{b\}]} p(a). \quad (2.3.2)$$

This functor can easily be modified by changing the set given in Equation (2.3.1). On the one hand we can enlarge it by considering *subdistributions*, i.e., functions $p: A \rightarrow [0, 1]$ where $\sum_{a \in A} p(a) \leq 1$ and on the other hand we can make it smaller by requiring that each (sub-)distribution has finite support, i.e., that the set $\text{supp}(p) := \{a \in A \mid p(a) > 0\}$ is finite. In analogy to the powerset functor will denote the latter functor by \mathcal{D}_f .

Having seen these examples we quickly note that the composition of functors is again a functor. The proof is easy and hence omitted.

Lemma 2.3.13 (Composed Functor) Let \mathcal{C} , \mathcal{D} and \mathcal{E} be arbitrary categories and $F: \mathcal{C} \rightarrow \mathcal{D}$ and $G: \mathcal{D} \rightarrow \mathcal{E}$ be functors. If we define $HA := G(FA)$ for all \mathcal{C} -objects A and $Hf := G(Ff)$ for all $f \in \mathcal{A}(\mathcal{C})$ we obtain a functor $H: \mathcal{C} \rightarrow \mathcal{E}$. Instead of H we also write $G \circ F$ or simply GF .

In the light of the previous result, we briefly remark that the small categories and the functors between them give rise to a new category, which we denote by Cat . Taking proper care of the involved sizes, we can even define a quasicategory (which is essentially the same as a category but both objects and arrows may be larger than a class, i.e., conglomerates) of all categories.

Each functor between two categories immediately induces another functor between their dual categories, the so-called *opposite functor*.

Definition 2.3.14 (Opposite Functor) If $F: \mathcal{C} \rightarrow \mathcal{D}$ is a functor, then its opposite functor is the functor $F^{\text{op}}: \mathcal{C}^{\text{op}} \rightarrow \mathcal{D}^{\text{op}}$ given by the assignments $F^{\text{op}}A = FA$ for all $A \in \mathcal{C}^{\text{op}}$, and $F_{A,B}^{\text{op}}f = F_{B,A}f$ for all $f \in \mathcal{C}^{\text{op}}(A, B)$.

Having seen this, we quickly remark that we will later – especially in Chapter 5 – call a functor $F: \mathcal{C} \times \mathcal{D} \rightarrow \mathcal{E}$ where $\mathcal{C} \times \mathcal{D}$ is the product category of \mathcal{C} and \mathcal{D} (see Definition 2.3.9) a *bifunctor*. This naturally extends to functors whose domain of definition is the product of finitely many categories. We will thus call them *multifunctors*.

We close this section with some useful properties a functor can possess.

Definition 2.3.15 (Full, Faithful, Fully Faithful) We call a functor $F: \mathcal{C} \rightarrow \mathcal{D}$

1. *faithful* if for all \mathcal{C} -objects A, B the function $F_{A,B}$ is injective.

2. *full* if for all \mathcal{C} -objects A, B the function $F_{A,B}$ is surjective.
3. *fully faithful* if for all \mathcal{C} -objects A, B the function $F_{A,B}$ is bijective.

2.3.3 Limits and Colimits

The strength of category theory lies in its abstraction from certain details. Many categorical constructions thus make use of the concept of *universal properties*. If we want to define something (usually an object together with some arrows) we just say what properties it should satisfy and require that it does that in a universal manner. Plenty of examples of such a definition arise as so-called *limits* or dually *colimits*.

Basic Definitions

In order to define limits and colimits, it is helpful to introduce the concept of a *diagram*, which is nothing but a new name for a functor.

Definition 2.3.16 (Diagram) Let \mathcal{I} and \mathcal{C} be arbitrary categories. A *diagram of type (or shape) \mathcal{I}* is a functor $D: \mathcal{I} \rightarrow \mathcal{C}$. In this context, the category \mathcal{I} is also called *index category*. Moreover, we call D a *small [finite]* diagram if \mathcal{I} is a small [finite] category.

A diagram with index category $(\circ \leftarrow \circ \rightarrow \circ)$ is called a *span* and a diagram with index category $(\circ \rightarrow \circ \leftarrow \circ)$ a *cospan*. Other diagrams which we will consider in the sequel are e.g. the unique diagram $\emptyset \rightarrow \mathcal{C}$ and diagrams with discrete index categories.

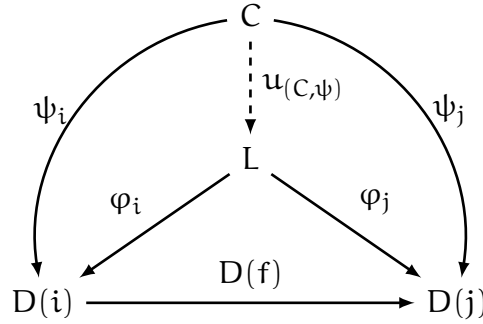
With this new name for functors we can now define *cones* and *limits*.

Definition 2.3.17 (Cone, Limit) Let $D: \mathcal{I} \rightarrow \mathcal{C}$ be a diagram. A *cone (to D)* is a tuple (C, ψ) consisting of a \mathcal{C} -object C together with a family of morphisms $\psi_i: C \rightarrow D(i)$ for each object i of \mathcal{I} such that each triangle (hence the name cone) of the following form commutes for all \mathcal{I} -objects i, j and every $f \in \mathcal{I}(i, j)$.

$$\begin{array}{ccc}
 & C & \\
 \psi_i \swarrow & & \searrow \psi_j \\
 D(i) & \xrightarrow{D(f)} & D(j)
 \end{array}$$

We call a cone (L, φ) a *weak limit (or weak limit cone)* if it is *weakly universal* in the sense that for any cone (C, ψ) there is an arrow $u_{(C, \psi)}: C \rightarrow L$ such that the

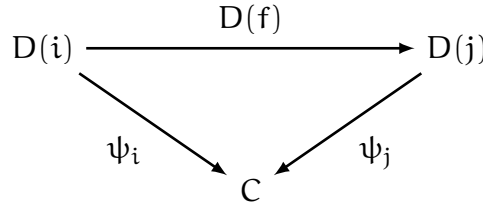
following diagram commutes for any $i, j \in \mathcal{I}$ and any $f \in \mathcal{I}(i, j)$.



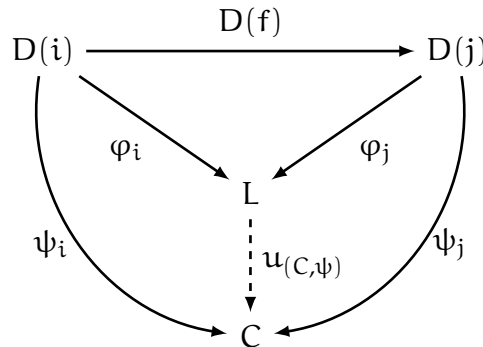
If (L, φ) is *universal*, i.e., if $u_{(C, \psi)}$ is always unique, we call it a *limit* (or *limit cone*). Moreover, we call a (weak) limit *small* [*finite*] if \mathcal{I} is a small [*finite*] category.

Before looking at examples of cones and limits, we *dualize* this notion, i.e., we turn all the arrows around to obtain *cocones* and *colimits*.

Definition 2.3.18 (Cocone, Colimit) Let $D: \mathcal{I} \rightarrow \mathcal{C}$ be a diagram. A *cocone* (from D) is a tuple (C, ψ) consisting of a \mathcal{C} -object C together with a family of morphisms $\psi_i: D(i) \rightarrow C$ for each object i of \mathcal{I} such that each triangle of the following form commutes for all \mathcal{I} -objects i, j and every $f \in \mathcal{I}(i, j)$.



We call a cocone (L, φ) a *weak colimit* (or *weak colimit cocone*) if it is weakly universal in the sense that for any cocone (C, ψ) there is an arrow $u_{(C, \psi)}: L \rightarrow C$ such that the following diagram commutes for any $i, j \in \mathcal{I}$ and any $f \in \mathcal{I}(i, j)$.



If (L, φ) is universal, i.e., if $u_{(C, \psi)}$ is always unique, we call it a *colimit* (or *colimit cocone*). Moreover, we call a colimit *small* [*finite*] if \mathcal{I} is a small [*finite*] category.

Neither limits nor colimits need to exist. However, if they do, it is easy to see that they are unique up to isomorphism. Categories in which all small limits exist, are called *complete* and categories in which all small colimits exist are called *cocomplete*. If a category is both complete and cocomplete, it is said to be *bicomplete*. An example for such a bicomplete category is *Set*.

Instances of Limits and Colimits

Let us now look at a few special instances of limits and colimits.

Definition 2.3.19 (Initial, Terminal and Zero Objects) Let \mathcal{C} be a category. We call an object A

1. an *initial object* if for every \mathcal{C} -object X there is a unique arrow $i_X: A \rightarrow X$,
2. a *final* (or *terminal*) *object* if for every \mathcal{C} -object X there is a unique arrow $f_X: X \rightarrow A$, or
3. a *zero object* if it is both an initial object and a terminal object.

This definition is indeed an example of both a limit and a colimit. If we consider the diagram given by the unique, empty functor $\emptyset \rightarrow \mathcal{C}$ then the object of its limit (if it exists) is precisely a final object of \mathcal{C} and the object of the colimit (if it exists) is an initial object.

Conversely, if for any given diagram D we consider the category $\mathbf{Cone}(D)$ whose objects are cones to D and whose morphisms are cone morphisms (i.e., morphisms like $u_{(C, \psi)}$ in Definition 2.3.17 (Cone, Limit) making the respective “triangles” commute) a limit is a final object in $\mathbf{Cone}(D)$. Analogously, a colimit is an initial object in a category $\mathbf{Cocone}(D)$ of cocones from D (consult the book *Category Theory* [Awo06, p. 89ff] for a detailed analysis of these connections).

In the category *Set* there is one unique initial object, the empty set \emptyset , and the final objects in *Set* are precisely the singletons. Thus there are no zero objects in *Set*.

Another instance of a limit is a product in a category.

Definition 2.3.20 (Product) Let I be an arbitrary class, \mathcal{C} be a category and $(X_i)_{i \in I}$ be a family of objects of \mathcal{C} indexed by I . We call an object X together with a family of arrows $(\pi_i: X \rightarrow X_i)_{i \in I}$ a *product* of the X_i , if for every other object Y together with a family of arrows $(f_i: Y \rightarrow X_i)_{i \in I}$ there is a unique arrow $f: Y \rightarrow X$ such that $\pi_i \circ f = f_i$ holds for all $i \in I$. If a product exists, we usually

denote the object X by $\prod_{i \in I} X_i$, the unique arrow f by $\langle \dots, f_i, \dots \rangle$ and call the π_i *projections*. This situation is summarized in the diagram below.

$$\begin{array}{ccc}
 & Y & \\
 & \downarrow f = \langle \dots, f_i, \dots \rangle & \\
 \prod_{i \in I} X_i & \xrightarrow{\pi_i} & X_i
 \end{array}$$

We call a product *small [finite]* if I is a set [finite]. For finite products we also write $\prod_{i=1}^n X_i$ or $X_1 \times \dots \times X_n$ instead of $\prod_{i \in \{1, \dots, n\}} X_i$.

We quickly check that this is indeed a limit. If we take the discrete category \mathcal{I} whose object class is I and the diagram $D: \mathcal{I} \rightarrow \mathcal{C}$ mapping $i \in \mathcal{I}$ to $X_i \in \mathcal{C}$ (and identities to identities), a product is just a limit object of this diagram (if it exists). Similarly, by considering the colimit (if it exists) of this diagram, we obtain the dual notion of coproduct.

Definition 2.3.21 (Coproduct) Let I be an arbitrary class, \mathcal{C} be a category and $(X_i)_{i \in I}$ be a family of objects of \mathcal{C} indexed by I . We call an object X together with a family of arrows $(\iota_i: X_i \rightarrow X)_{i \in I}$ a *coproduct* of the X_i , if for every other object Y together with a family of arrows $(f_i: X_i \rightarrow Y)_{i \in I}$ there is a unique arrow $f: X \rightarrow Y$ such that $f \circ \iota_i = f_i$ holds for all $i \in I$. If a coproduct exists, we usually denote the object X by $\coprod_{i \in I} X_i$, the unique arrow f by $[\dots, f_i, \dots]$ and call the ι_i *injections*. This situation is summarized in the diagram below.

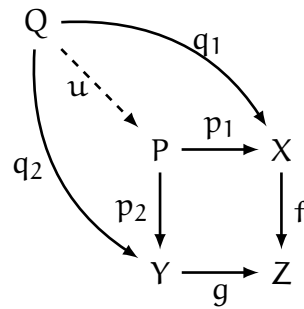
$$\begin{array}{ccc}
 X_i & \xrightarrow{\iota_i} & \coprod_{i \in I} X_i \\
 & \searrow f_i & \downarrow [\dots, f_i, \dots] = f \\
 & & Y
 \end{array}$$

We call a coproduct *small [finite]* if I is a set [finite]. For finite coproducts we also write $\coprod_{i=1}^n X_i$ or $X_1 + \dots + X_n$ instead of $\coprod_{i \in \{1, \dots, n\}} X_i$.

As is the case with general limits/colimits, neither products nor coproducts need to exist. In \mathbf{Set} all small products and coproducts exist and correspond to the usual cartesian products of sets and the disjoint union of sets respectively. Also the product of two small categories as defined in Definition 2.3.9 is an instance of a product in the category \mathbf{Cat} of all small categories and functors between them.

The last examples of limits/colimits we will consider are those of spans and cospans. However, we will just give an explicit definition of the latter (since only this is relevant for our purposes) and merely note, that the dual notion is called a *(weak) pushout*.

Definition 2.3.22 (Pullback and Weak Pullback) Let \mathcal{C} be a category. A *weak pullback* of two arrows $f: X \rightarrow Z$, $g: Y \rightarrow Z$ is an object P together with arrows $p_1: P \rightarrow X$, $p_2: P \rightarrow Y$ satisfying $f \circ p_1 = g \circ p_2$ such that for any other object Q along with arrows $q_1: Q \rightarrow X$, $q_2: Q \rightarrow Y$ satisfying $f \circ q_1 = g \circ q_2$ there is an arrow $u: Q \rightarrow P$ satisfying $q_1 = p_1 \circ u$ and $q_2 = p_2 \circ u$. This situation is depicted in the following diagram.



If u is always unique we call (P, p_1, p_2) a *pullback* of f and g . In this case we denote P by $X \times_Z Y$.

Since we will use them later, let us briefly consider pullbacks in \mathbf{Set} .

Example 2.3.23 (Pullbacks in \mathbf{Set}) Let X, Y, Z be sets and $f: X \rightarrow Z$, $g: Y \rightarrow Z$ be functions. The pullback of f and g is the set

$$X \times_Z Y := \{(x, y) \in X \times Y \mid f(x) = g(y)\}$$

together with the restricted projections of the product $\pi_X|_{X \times_Z Y}$ and $\pi_Y|_{X \times_Z Y}$.

Limit and Colimit Preserving Functors

The last part of this section is devoted to functors that behave well with respect to limits/colimits.

Definition 2.3.24 (Limit/Colimit Preserving) We say a functor $F: \mathcal{C} \rightarrow \mathcal{D}$ *preserves (weak) limits* for diagrams of type \mathcal{J} if for every (weak) limit (L, φ) to a diagram $D: \mathcal{J} \rightarrow \mathcal{C}$ the cone⁵ $(FL, F\varphi)$ is a (weak) limit to the diagram $FD: \mathcal{J} \rightarrow \mathcal{D}$.

⁵where $F\varphi$ represents the family of arrows $F\varphi_i: FL \rightarrow FD(i)$

If for every limit (L, φ) to a diagram $D: \mathcal{I} \rightarrow \mathcal{C}$ the cone $(FL, F\varphi)$ is a weak limit to the diagram $FD: \mathcal{I} \rightarrow \mathcal{D}$ we say F *weakly preserves limits* of type \mathcal{I} .

Dually, a functor $F: \mathcal{C} \rightarrow \mathcal{D}$ *preserves (weak) colimits* for diagrams of type \mathcal{I} if for every (weak) colimit (L, φ) from a diagram $D: \mathcal{I} \rightarrow \mathcal{C}$ the cocone $(FL, F\varphi)$ is a (weak) colimit from the diagram $FD: \mathcal{I} \rightarrow \mathcal{D}$. If for every colimit (L, φ) from a diagram $D: \mathcal{I} \rightarrow \mathcal{C}$ the cocone $(FL, F\varphi)$ is a weak colimit from the diagram $FD: \mathcal{I} \rightarrow \mathcal{D}$ we say F *weakly preserves colimits* of type \mathcal{I} .

We will often be interested in functors that preserve (weak) pullbacks. In such a situation the following results are useful.

Lemma 2.3.25 ([Gum01, Lemma 2.6]) Let \mathcal{C} be a category in which all pullbacks exist and let $F: \mathcal{C} \rightarrow \mathcal{C}$ be a functor. Then the following are equivalent:

1. F preserves weak pullbacks.
2. F weakly preserves pullbacks.

Since clearly every pullback is also a weak pullback, we can easily deduce another result.

Corollary 2.3.26 ([Rutoo, Proposition A.4]) Let \mathcal{C} be a category in which all pullbacks exist and let $F: \mathcal{C} \rightarrow \mathcal{C}$ be a functor. If F preserves pullbacks then F preserves weak pullbacks.

We conclude this section by remarking that the previous two results are certainly applicable to \mathbf{Set} – a property which we will use in Section 2.2.

2.3.4 Adjunctions and Monads

We will now proceed to some of the most important notions of category theory: adjunctions and monads. In order to define these, we will first have to consider so-called natural transformations.

Natural Transformations

Up until now we have considered categories and morphisms (functors) between them. As a next step we will consider morphisms between functors.

Definition 2.3.27 (Natural Transformation) Let $F, G: \mathcal{C} \rightarrow \mathcal{D}$ be functors. A *natural transformation* (from F to G), denoted $\alpha: F \Rightarrow G$, consists of a \mathcal{D} -arrow $\alpha_A: FA \rightarrow GA$ for each \mathcal{C} -object A such that the diagram below commutes for all \mathcal{C} -arrows $f: A \rightarrow B$.

$$\begin{array}{ccc}
 FA & \xrightarrow{Ff} & FB \\
 \alpha_A \downarrow & & \downarrow \alpha_B \\
 GA & \xrightarrow{Gf} & GB
 \end{array}$$

We call the α_A *components* of α and if all of them are isomorphisms, we call α a *natural isomorphism*.

A simple example of a natural transformation is the *identity natural transformation* Id_F from a functor $F: \mathcal{C} \rightarrow \mathcal{D}$ to itself. It consists of all the identity morphisms id_{FA} for every object $A \in \mathcal{C}$. Clearly, this is an example of a natural isomorphism. We will see more examples later.

Given two natural transformation, we can compose them to obtain a new one.

Lemma 2.3.28 (Composition of Natural Transformations) Let $F, G, H: \mathcal{C} \rightarrow \mathcal{D}$ be functors and $\alpha: F \Rightarrow G, \beta: G \Rightarrow H$ be natural transformations. We obtain a natural transformation $\beta\alpha: F \Rightarrow H$ by defining $(\beta\alpha)_A := \beta_A \circ \alpha_A: FA \rightarrow HA$ for all \mathcal{C} -objects A .

It is easy to see (and well-known) that this statement is true and moreover that the functors from \mathcal{C} to \mathcal{D} together with the natural transformations between them give rise to another quasicategory, the *functor (quasi-)category* $[\mathcal{C}, \mathcal{D}]$. It is a category if both \mathcal{C} and \mathcal{D} are small and isomorphic to a category if A is small and B is large [AHS90, Remark 6.16 (1)].

Whenever we have a natural transformation and an endofunctor we can obtain new natural transformations as follows. The proof of this lemma is easy and hence omitted.

Lemma 2.3.29 Let $F, G: \mathcal{C} \rightarrow \mathcal{D}$ be functors, and $\alpha: F \Rightarrow G$ a natural transformation.

1. For each functor $C: \mathcal{C} \rightarrow \mathcal{C}$ we obtain a natural transformation $\alpha C: FC \Rightarrow GC$ by defining $(\alpha C)_A = \alpha_{CA}$ for every \mathcal{C} -object A .
2. For each functor $D: \mathcal{D} \rightarrow \mathcal{D}$ we obtain a natural transformation $D\alpha: DF \Rightarrow DG$ by defining $(D\alpha)_A = D\alpha_A$ for every \mathcal{C} -object A .

Adjunctions

We now introduce one of the most important concepts of category theory. It describes a special relationship between two categories with two functors

between them in both directions. Before giving a formal definition we quickly look at the free monoid construction again and its universal property that we already mentioned in the Introduction. However, this time we will employ a category theoretic approach.

Example 2.3.30 (Universal Property of the Free Monoid Construction) We consider the categories \mathbf{Set} and \mathbf{Mon} of Examples 2.3.2 and 2.3.4. There is an apparent forgetful functor $R: \mathbf{Mon} \rightarrow \mathbf{Set}$ which maps a monoid to its underlying set. Moreover, there is also a functor $L: \mathbf{Set} \rightarrow \mathbf{Mon}$ in the other direction which maps each set A to the free monoid $(A^*, \text{conc}, \varepsilon)$ and each function $f: A \rightarrow B$ to the monoid homomorphism $f^*: A^* \rightarrow B^*$ where $f^*(\varepsilon) = \varepsilon$ and $f^*(a_1 \dots a_n) = f(a_1) \dots f(a_n)$ for all $a_1 \dots a_n \in A^*$.

Remembering the discussion from the Introduction, we recall that for every monoid (M, \circ, e) there is a bijection between functions $f: A \rightarrow M$ and monoid homomorphisms $h: (A^*, \text{conc}, \varepsilon) \rightarrow (M, \circ, e)$ satisfying $h(a) = f(a)$ for all $a \in A$. Explicitly, given a function f as above and any string $a_1 \dots a_n$ we define $h_f(a_1 \dots a_n) = f(a_1) \circ \dots \circ f(a_n)$ and conversely for any monoid homomorphism h as above and any element $a \in A$ we define $f_h(a) = h(a)$. From this we drew the conclusion that the free monoid construction can be seen as the *most efficient way* to turn an arbitrary set into a monoid which includes the initial set.

Employing a category theoretic notation we have a bijection between the set⁶ $\mathbf{Set}(A, M)$ of functions and the set $\mathbf{Mon}((A^*, \text{conc}, \varepsilon), (M, \circ, e))$ of monoid homomorphisms for all sets A and all monoids (M, \circ, e) . Using the functors from above we can write this as bijection $\mathbf{Set}(A, R(M, \circ, e)) \cong \mathbf{Mon}(LA, (M, \circ, e))$ which is the reason why we call the functors L and R *adjoint*.

Contrary to what this example suggests, we will use a definition of adjoint functors which uses two natural transformations called unit and counit. However, it can be shown that this definition induces a bijection as in the example above and conversely such a bijection (which has to satisfy additional constraints) yields the definition below [Awo06, Chapter 9].

Definition 2.3.31 (Adjunction, Adjoint Functors) Let \mathcal{C} and \mathcal{D} be categories. An *adjunction* between \mathcal{C} and \mathcal{D} consists of

- ▷ a functor $L: \mathcal{C} \rightarrow \mathcal{D}$, called *left adjoint*,
- ▷ a functor $R: \mathcal{D} \rightarrow \mathcal{C}$, called *right adjoint*,

⁶Recall that \mathbf{Set} is locally small so that we have indeed a set and not a proper class. The same is true for \mathbf{Mon} .

- ▷ a natural transformation $\eta: \text{Id}_{\mathcal{C}} \Rightarrow \text{RL}$, called *unit*, and
 - ▷ a natural transformation $\varepsilon: \text{LR} \Rightarrow \text{Id}_{\mathcal{D}}$, called *counit*,
- such that the following two diagrams commute⁷.

$$\begin{array}{ccc}
 L & \xrightarrow{L\eta} & \text{LRL} \\
 & \searrow \text{Id}_L & \downarrow \varepsilon L \\
 & & L
 \end{array}
 \qquad
 \begin{array}{ccc}
 R & \xrightarrow{\eta R} & \text{RLR} \\
 & \searrow \text{Id}_R & \downarrow R\varepsilon \\
 & & R
 \end{array}
 \tag{2.3.3}$$

We denote such an adjunction by $(L \dashv R, \eta, \varepsilon): \mathcal{C} \rightarrow \mathcal{D}$. A functor $L: \mathcal{C} \rightarrow \mathcal{D}$ [$R: \mathcal{D} \rightarrow \mathcal{C}$] is a *left adjoint* [*right adjoint*] if it is the left adjoint [right adjoint] of some adjunction $(L \dashv R, \eta, \varepsilon): \mathcal{C} \rightarrow \mathcal{D}$.

The convention of calling a functor left adjoint [right adjoint] without giving the full adjunction is justified because one can prove that the functor determines the other parts of the adjunction uniquely up to isomorphism. However, since this is not trivial, we will always give the full adjunction.

In order to see that the free monoid construction of Example 2.3.30 is indeed captured by this definition we provide the unit and counit. As we have briefly discussed in the Introduction, for any set A there is the function $\eta_A: A \rightarrow A^*$ mapping each letter $a \in A$ to itself, interpreted as an element of A^* . Moreover, for any monoid (M, \circ, e) , we can define a monoid homomorphism $\varepsilon_{(M, \circ, e)}: M^* \rightarrow M$ by defining $\varepsilon_{(M, \circ, e)}(\varepsilon) = e$ and $\varepsilon_{(M, \circ, e)}(m_1 m_2 \dots m_n) = m_1 \circ m_2 \circ \dots \circ m_n$ for all words $m_1 m_2 \dots m_n \in M^*$.

Since we will encounter many other concrete examples of adjunctions in Chapter 3 we just consider one other (standard) example.

Example 2.3.32 Let $L: \text{Set} \rightarrow \text{Rel}$ be the inclusion functor from Set to Rel mapping each set X to itself and each function $f: X \rightarrow Y$ to the corresponding relation $f: X \leftrightarrow Y$. Moreover, let $R: \text{Rel} \rightarrow \text{Set}$ be the functor which maps each set X to its powerset $\mathcal{P}X$ and each relation $f: X \leftrightarrow Y$ to the function

$$Rf: \mathcal{P}X \rightarrow \mathcal{P}Y, \quad (Rf)(S) = \{y \in Y \mid \exists x \in S : (x, y) \in f\}. \tag{2.3.4}$$

We obtain an adjunction $(L \dashv R, \eta, \varepsilon): \text{Set} \rightarrow \text{Rel}$ where the unit $\eta: \text{Id}_{\text{Set}} \Rightarrow \mathcal{P}$ is

⁷In these diagrams we use the notation introduced in Lemma 2.3.29. A diagram involving natural transformations obviously induces a family of diagrams by considering the components of the natural transformation. Commutativity of such a diagram is thus given if and only if each of these induced diagrams commutes.

given by the functions

$$\eta_X: X \rightarrow \mathcal{P}X, \quad \eta_X(x) = \{x\} \quad (2.3.5)$$

for every set X and the counit $\varepsilon: \mathcal{P} \Rightarrow \text{Id}_{\text{Rel}}$ consists of the relations

$$\varepsilon_X: \mathcal{P}X \leftrightarrow X \quad (S, x) \in \varepsilon_X \iff x \in S \quad (2.3.6)$$

for every set X .

There are special instances of adjunctions which have their own names.

Definition 2.3.33 (Equivalence and Duality of Categories)

1. We call an adjunction $(L \dashv R, \eta, \varepsilon) : \mathcal{C} \rightarrow \mathcal{D}$ an *equivalence (of categories)* if both η and ε are natural isomorphisms. Whenever such an equivalence exists, we say that the categories \mathcal{C} and \mathcal{D} are *equivalent*.
2. We call an equivalence $(L \dashv R, \varepsilon, \eta) : \mathcal{C} \rightarrow \mathcal{D}^{\text{op}}$ a *duality (of categories)*. Whenever such an equivalence exists, we say that the categories \mathcal{C} and \mathcal{D} are *dually equivalent*.

Monads

For the coalgebraic definition of traces we will need another categorical construct that arises uniquely from an adjunction, a so-called *monad*.

Definition 2.3.34 (Monad) A monad on an arbitrary category \mathcal{C} is a triple (T, η, μ) where $T: \mathcal{C} \rightarrow \mathcal{C}$ is an endofunctor and $\eta: \text{Id} \Rightarrow T$, $\mu: T^2 \Rightarrow T$ are natural transformations called *unit* (η) and *multiplication* (μ) such that the two diagrams below commute.

$$\begin{array}{ccc} T & \xrightarrow{\eta T} & T^2 \\ & \searrow \mu & \swarrow T\eta \\ & T & \end{array} \qquad \begin{array}{ccc} & T^3 & \xrightarrow{\mu T} & T^2 \\ T\mu \downarrow & & & \downarrow \mu \\ T^2 & \xrightarrow{\mu} & T & \end{array}$$

We claimed that each adjunction $(L \dashv R, \eta, \varepsilon) : \mathcal{C} \rightarrow \mathcal{D}$ gives rise to a monad. Indeed, one can check that the tuple $(RL, \eta, R\varepsilon L)$ satisfies the above axioms. If we do this with our adjunction from Example 2.3.32, we obtain the powerset monad.

Example 2.3.35 (Powerset Monad) The powerset functor \mathcal{P} of Example 2.3.11 and its finite variants can be seen as a monad. The unit η consists of the functions $\eta_X: X \rightarrow \mathcal{P}X$, $\eta_X(x) = \{x\}$ and the multiplication is given by $\mu_X: \mathcal{P}\mathcal{P}X \rightarrow \mathcal{P}X$, $\mu_X(S) = \cup S$.

Even though we did not consider an adjunction involving probability distributions, we can still check that also the distribution functors are part of a monad.

Example 2.3.36 (Distribution Monad) The probability distribution functor \mathcal{D} of Example 2.3.12 and its variants can be seen as a monad: the unit η consists of the functions $\eta_X: X \rightarrow \mathcal{D}X$, $\eta_X(x) = \delta_x^X$ where $\delta_x^X: X \rightarrow [0, 1]$ is the Dirac distribution (where $\delta_x^X(y) = 1$ if $y = x$ and 0 otherwise) and the multiplication is given by $\mu_X: \mathcal{D}\mathcal{D}X \rightarrow \mathcal{D}X$, $\mu_X(P) = \lambda x. \sum_{q \in \mathcal{D}X} P(q) \cdot q(x)$.

The Kleisli Category

If we are in a case as in the previous example, where we are given a monad (T, η, μ) on a category \mathcal{C} without an adjunction to start from, it is a legitimate question to ask whether we can construct an adjunction giving rise to that monad. For this we need a category \mathcal{D} and an adjunction $(L \dashv R, \eta', \varepsilon): \mathcal{C} \rightarrow \mathcal{D}$ such that $T = RL$, $\eta = \eta'$ and $\mu = R\varepsilon L$. With the proper notion of *adjunction morphism* [Mac98, page 99] the adjunctions giving rise to the monad form a (quasi-)category. This category has both initial and final objects [Mac98, Theorem VI.5.3]. We start by describing the category belonging to the initial object.

Definition 2.3.37 (Kleisli Category) Let (T, η, μ) be a monad on a category \mathcal{C} . The *Kleisli category* of T , which we denote by $\mathcal{Kl}(T)$, has the same objects as \mathcal{C} . For any two objects X and Y , a Kleisli arrow $f: X \rightsquigarrow Y$ is a \mathcal{C} -arrow $f: X \rightarrow TY$, i.e., we define $\mathcal{Kl}(T)(X, Y) = \mathcal{C}(X, TY)$. The identity arrow for any Kleisli object X is $\eta_X: X \rightarrow TX$. Composition of Kleisli arrows $f: X \rightarrow TY$ and $g: Y \rightarrow TZ$ is defined as $g \circ_T f := \mu_Z \circ T(g) \circ f$.

Note that in this definition we used the same symbol f for both the Kleisli arrow $f: X \rightsquigarrow Y$ as well as the underlying \mathcal{C} -arrow $f: X \rightarrow TY$. We will do this frequently in this thesis.

The adjunction between the base category \mathcal{C} and the Kleisli-category $\mathcal{Kl}(T)$ which gives rise to the monad (T, η, μ) is the following.

Definition 2.3.38 (Kleisli Adjunction) Let (T, η, μ) be a monad. The *Kleisli adjunction* $(L_T \dashv R_T, \eta, \varepsilon) : \mathcal{C} \rightarrow \mathcal{Kl}(T)$ is given by the following ingredients.

- ▷ The left adjoint $L_T : \mathcal{C} \rightarrow \mathcal{Kl}(T)$ maps each object to itself and an arrow $f : X \rightarrow Y$ to the Kleisli-arrow $\eta_Y \circ f : X \rightsquigarrow Y$ (i.e., the \mathcal{C} -arrow $\eta_Y \circ f : X \rightarrow TY$).
- ▷ The right adjoint $R_T : \mathcal{Kl}(T) \rightarrow \mathcal{C}$, maps each Kleisli object X to TX and each Kleisli-arrow $f : X \rightsquigarrow Y$ (i.e., a \mathcal{C} -arrow $f : X \rightarrow TY$) to $\mu_Y \circ Tf : TX \rightarrow TY$.
- ▷ The unit of the adjunction is the unit of the monad.
- ▷ The counit consists of the Kleisli arrows $\varepsilon_Y : TY \rightsquigarrow Y$ which correspond to the identities $\text{id}_{TY} : TY \rightarrow TY$ for an arbitrary Kleisli object Y .

As an example we instantiate the above definition to the powerset monad. We obtain the following category.

Example 2.3.39 (The Kleisli Category of the Powerset Monad) The Kleisli category of the powerset monad has as objects the class of all sets and a morphism $X \rightsquigarrow Y$ corresponds to a function $f : X \rightarrow \mathcal{P}Y$. Any such function can equivalently be expressed as a relation $R_f : X \leftrightarrow Y$ by defining $R_f := \{(x, y) \mid x \in X, y \in f(x)\}$ and conversely any relation $R : X \leftrightarrow Y$ can be turned into the function $f_R : X \rightarrow \mathcal{P}Y$ by defining $f_R(x) := \{y \in Y \mid (x, y) \in R\}$. Thus $\mathcal{Kl}(\mathcal{P})$ is isomorphic to the category Rel of sets and relations.

The Eilenberg-Moore Category

Let us now consider the category belonging to the final object of the quasicategory of adjunctions giving rise to a monad.

Definition 2.3.40 (Eilenberg-Moore Algebra and Eilenberg-Moore Category)

An *Eilenberg-Moore algebra* for a monad (T, η, μ) on a category \mathcal{C} is a \mathcal{C} -arrow $a : TA \rightarrow A$ making the left and middle diagram below commute. We will sometimes call A the *carrier* of the algebra a and conversely call a the *structure (map)* on A . Given two algebras $a : TA \rightarrow A$ and $b : TB \rightarrow B$, a morphism from a to b is a \mathcal{C} arrow $f : A \rightarrow B$ making the right diagram below commute.

$$\begin{array}{ccc}
 \begin{array}{ccc} A & \xrightarrow{\eta_A} & TA \\ & \searrow \text{id}_A & \downarrow a \\ & & A \end{array} &
 \begin{array}{ccc} T^2A & \xrightarrow{\mu_A} & TA \\ T a \downarrow & & \downarrow a \\ TA & \xrightarrow{a} & A \end{array} &
 \begin{array}{ccc} TA & \xrightarrow{Tf} & TB \\ a \downarrow & & \downarrow b \\ A & \xrightarrow{f} & B \end{array}
 \end{array}$$

The Eilenberg-Moore algebras and their morphisms form a category which we denote by $\mathcal{EM}(T)$.

It is easy to see that each component $\mu_X: TTX \rightarrow TX$ of the multiplication of the monad is an example of an Eilenberg-Moore algebra. It is called the *free algebra (on X)*. As before, we consider the corresponding adjunction.

Definition 2.3.41 (Eilenberg-Moore Adjunction) Let (T, η, μ) be a monad. The Eilenberg-Moore adjunction $(L^T \dashv R^T, \eta, \epsilon): \mathcal{C} \rightarrow \mathcal{EM}(T)$ is given by the following ingredients.

- ▷ The left adjoint $L^T: \mathcal{C} \rightarrow \mathcal{EM}(T)$ maps each object of \mathcal{C} to its free algebra $\mu_X: TTX \rightarrow TX$ and an arrow $f: X \rightarrow Y$ to the algebra homomorphism $Tf: TX \rightarrow TY$.
- ▷ The right adjoint $R^T: \mathcal{EM}(T) \rightarrow \mathcal{C}$ maps each algebra $a: TA \rightarrow A$ to its carrier A and each algebra homomorphism $f: (a: TA \rightarrow A) \rightarrow (b: TB \rightarrow B)$ to the underlying \mathcal{C} -arrow $f: A \rightarrow B$.
- ▷ The unit of the adjunction is the unit of the monad.
- ▷ The components of the counit are given by the assignment $\epsilon_{(a: TA \rightarrow A)} := a$ for each algebra $a: TA \rightarrow A$.

Liftings and Extensions

For our later results we will have to define functors on Kleisli and Eilenberg-Moore categories which are based on a functor F on the base category. We will use the following terminology.

Definition 2.3.42 (Lifting, Extension) Let $(L \dashv R, \eta, \epsilon): \mathcal{C} \rightarrow \mathcal{D}$ be an adjunction and F be an endofunctor on \mathcal{C} . We call an endofunctor G on \mathcal{D}

1. an *extension* of F if $GL = LF$,
2. a *lifting* of F if $RG = FR$.

This terminology can easily be understood if one has a forgetful functor as right adjoint and a kind of embedding as left adjoint. Please note that many authors do not differentiate between extensions and liftings and simply call both a *lifting*.

In order to obtain liftings or extensions of functors, we can make use of certain natural transformations which are called *distributive laws*.

Definition 2.3.43 (Distributive Laws) Let F be an endofunctor and (T, η, μ) be a monad on a category \mathcal{C} .

1. We call a natural transformation $\lambda: TF \Rightarrow FT$ an *Eilenberg-Moore law* or short *EM-law* if the following diagrams commute.

$$\begin{array}{ccc} F & & \\ \eta F \downarrow & \searrow F\eta & \\ TF & \xrightarrow{\lambda} & FT \end{array}$$

$$\begin{array}{ccccc} T^2F & \xrightarrow{T\lambda} & TFT & \xrightarrow{\lambda T} & FT^2 \\ \mu F \downarrow & & & & \downarrow F\mu \\ TF & \xrightarrow{\lambda} & & & FT \end{array}$$

2. We call a natural transformation $\lambda: FT \Rightarrow TF$ a *Kleisli law* or short *Kl-law* if the following diagrams commute.

$$\begin{array}{ccc} F & & \\ F\eta \downarrow & \searrow \eta F & \\ FT & \xrightarrow{\lambda} & TF \end{array}$$

$$\begin{array}{ccccc} FT^2 & \xrightarrow{\lambda T} & TFT & \xrightarrow{T\lambda} & T^2F \\ F\mu \downarrow & & & & \downarrow \mu F \\ FT & \xrightarrow{\lambda} & & & TF \end{array}$$

If it is clear from the context which of the two above definitions is meant, we will sometimes just call λ a *distributive law*.

As stated before, distributive laws are closely related to liftings and extensions as the following, well-known result shows.

Theorem 2.3.44 (Distributive Laws, Extensions and Liftings) Let (T, η, μ) be a monad and F be an endofunctor on a common category \mathcal{C} .

1. Extensions $G: \mathcal{Kl}(T) \rightarrow \mathcal{Kl}(T)$ of F to the Kleisli category of the monad are in one-to-one correspondence with \mathcal{Kl} -laws $\lambda: FT \rightarrow TF$ [Joh75, Lemma 1], [JSS15, Proposition 1].
2. Liftings $G: \mathcal{EM}(T) \rightarrow \mathcal{EM}(T)$ of F to the Eilenberg-Moore category of the monad are in one-to-one correspondence with \mathcal{EM} -laws $\lambda: TF \rightarrow FT$ [Mul94, Theorem 2.2].

With this theoretical result in place we finish our short excursion to the general category theoretical background needed for understanding this thesis.

2.4 Coalgebra

After our short recap of transition system theory and the earlier introduction to category theory, we are now able to combine both and discuss coalgebra. While the definition of a coalgebra itself is very simple, coalgebras and their homomorphisms provide a suitable framework to model many kinds of transition systems. As before, we will just provide the basic definitions and results needed to understand the subsequent parts of this thesis. The interested reader is invited to read Bart Jacobs' and Jan Rutten's tutorial paper [JR97] as well as Jan Rutten's detailed fundamental study [Rutoo] from which we have taken some of the results.

2.4.1 Coalgebras are Transition Systems

Recall that in Definition 2.3.40 we have defined an algebra for a monad (T, η, μ) as an arrow $\alpha: TA \rightarrow A$ satisfying additional commutativity requirements involving the unit and counit of the monad. If we drop these requirements and allow an arbitrary endofunctor F , we obtain the definition of an *algebra* for an endofunctor. As the name suggests, a coalgebra is just the categorical dual to this which we obtain by turning around the arrow.

Definition 2.4.1 (Coalgebra, Coalgebra Homomorphism) Let F be an endofunctor on a category \mathcal{C} . An F -coalgebra is a \mathcal{C} -arrow $\alpha: A \rightarrow FA$. Given another F -coalgebra $b: B \rightarrow FB$, an F -coalgebra homomorphism from α to b is a \mathcal{C} -arrow $f: A \rightarrow B$ such that the diagram below commutes.

$$\begin{array}{ccc} A & \xrightarrow{f} & B \\ \alpha \downarrow & & \downarrow b \\ FA & \xrightarrow{Ff} & FB \end{array}$$

We use the same symbol f for both the F -coalgebra homomorphism $f: \alpha \rightarrow b$ and the underlying \mathcal{C} -arrow $f: A \rightarrow B$. Moreover, if the functor F is clear from the context we will use the terms *coalgebra* and *coalgebra homomorphism*.

As a simple first example we consider the category of sets and functions and the powerset functor $\mathcal{P}: \text{Set} \rightarrow \text{Set}$ of Example 2.3.11. A coalgebra $s: X \rightarrow \mathcal{P}X$ of this functor corresponds to an unlabelled transition system. The function s maps each state $x \in X$ to the set $s(x) \subseteq X$ of its successors.

Apparently the function $s: X \rightarrow \mathcal{P}X$ corresponds to an endorelation, i.e., a relation $R \subseteq X \times X$ whose domain and codomain coincide. These relations are the coalgebras for the identity functor $\text{Id}_{\text{Rel}}: \text{Rel} \rightarrow \text{Rel}$ on the category of sets and relations. Thus we have just found an alternative coalgebraic model of unlabelled transition systems.

In order to model labelled transition systems, we introduce another functor, the so-called input functor.

Example 2.4.2 (Input Functor) Let A be an arbitrary set. The *input functor* $F = _{}^A: \text{Set} \rightarrow \text{Set}$ maps a set X to the set X^A of all functions $A \rightarrow X$ and a function $f: X \rightarrow Y$ to $f^A: X^A \rightarrow Y^A$, $f^A(g) = f \circ g$.

A coalgebra $s: X \rightarrow X^A$ for this functor corresponds to a *deterministic* labelled transition system where for each state $x \in X$ and each *input* $a \in A$ the function s selects $s(x)(a) \in X$ as *unique* a -successor of x .

In order to model arbitrary LTS, we have to combine the input functor with the powerset functor from Example 2.3.11. We need to consider coalgebras for the functor $(\mathcal{P}_)^A: \text{Set} \rightarrow \text{Set}$ which is just the composition $_{}^A \circ \mathcal{P}$ of the two functors. Indeed, a coalgebra $c: X \rightarrow (\mathcal{P}X)^A$ is nothing but a labelled transition system. For each state $x \in X$ and each action $a \in A$ the set $c(x)(a) \in \mathcal{P}(X)$ is the set of all a -successors of x . We can recover the transition relation by defining $\rightarrow := \{(x, a, y) \mid x \in X, a \in A, y \in c(x)(a)\}$ and conversely any transition relation $\rightarrow \subseteq X \times A \times X$ can be transformed into such a coalgebra by defining $c(x)(a) := \{y \in X \mid (x, a, y) \in \rightarrow\}$.

Using this example let us carefully examine which functions are coalgebra homomorphisms⁸. Given an LTS $c: X \rightarrow (\mathcal{P}X)^A$ and another system $d: Y \rightarrow (\mathcal{P}Y)^A$, a function $f: X \rightarrow Y$ between their state spaces is a coalgebra homomorphism provided that $(f[\cdot])^A \circ c = d \circ f$. A short and elementary calculation yields that this is equivalent to

$$\left\{ f(x') \mid x \xrightarrow{a} x' \right\} = f[c(x)(a)] = d(f(x))(a) = \left\{ y' \mid f(x) \xrightarrow{a} y' \right\}$$

for every $x \in X$ and every $a \in A$. Thus

1. for every transition $x \xrightarrow{a} x'$ in the first system, we must have the transition $f(x) \xrightarrow{a} f(x')$ in the second system, and conversely
2. for every transition $f(x) \xrightarrow{a} y'$ in the second system, we must have a transition $x \xrightarrow{a} x'$ in the first system with $f(x') = y'$.

⁸Jan Rutten explained this for LTS as coalgebras $c: X \rightarrow \mathcal{P}(A \times X)$ [Rutoo, Example 2.1].

Thus a coalgebra homomorphism is a function between the state spaces of two systems that preserves and reflects the transition structure.

The aforementioned model is not the only coalgebraic model of labelled transition systems. There is a formally completely equivalent alternative variant which, however, changes the interpretation a bit. As we have already discussed before, for an LTS we can think of the actions as something that allows the user to actively control the system, i.e., an action corresponds to something like pressing a button. This is captured by the above model where we consider coalgebras of the shape $c: X \rightarrow (\mathcal{P}X)^A$. Given a state x , the function $c(x): A \rightarrow \mathcal{P}X$ describes how the system reacts to the *inputs* $a \in A$.

Alternatively we can also imagine that a labelled transition system has no means of control (i.e., no input) but that its transitions are taken arbitrarily and whenever the system traverses a transition it *outputs* the label $a \in A$ of that transition. With this interpretation in mind we introduce another functor, which we thus call *output functor*.

Example 2.4.3 (Output Functor) Let A be a set. The functor $A \times _ : \text{Set} \rightarrow \text{Set}$ maps a set X to $FX = A \times X$ and a function $f: X \rightarrow Y$ to the function $Ff = \text{id}_A \times f$.

If we just consider the coalgebras of this functor, we obtain another version of deterministic LTS where from each state there is one unique transition. Alternatively we may interpret a coalgebra $c = \langle o, s \rangle: X \rightarrow A \times X$ as a transition system without transition labels where every *state* $x \in X$ has an *output value* (or a *state label*) $o(x)$ and a unique successor $s(x) \in X$.

As before we can combine this functor with the powerset functor from Example 2.3.11 to model arbitrary LTS. Here we consider coalgebras for endofunctor $\mathcal{P}(A \times _) = \mathcal{P} \circ (A \times _)$ on Set . Given such a coalgebra $c: X \rightarrow \mathcal{P}(A \times X)$, the set $c(x) \subseteq A \times X$ contains all the pairs of actions and states that are possible from the state x . Of course, as above we can recover the transition relation of the underlying transition system by defining $\rightarrow := \{(x, a, y) \mid (a, x) \in c(x)\}$ and conversely if we are given a transition relation we can define a coalgebra of the above type by letting $c(x) := \{(a, y) \mid (x, a, y) \in \rightarrow\}$.

The underlying mathematical reason for why we can equivalently model labelled transition systems as coalgebras of the shape $X \rightarrow (\mathcal{P}X)^A$ or of the shape $X \rightarrow \mathcal{P}(A \times X)$ is a property of the powerset. We quickly summarize some of these properties below.

Lemma 2.4.4 Let A, B be arbitrary sets. Then the following holds.

1. $\mathcal{P}A \cong 2^A$, in particular $\mathcal{P}1 \cong 2^1 \cong 2$
2. $\mathcal{P}(A + B) \cong \mathcal{P}A \times \mathcal{P}B$

$$3. \mathcal{P}(A \times B) \cong (\mathcal{P}A)^B \cong (\mathcal{P}B)^A$$

The proof of this lemma is a straightforward and simple calculation so we omit it here. Instead, we pick up the discussion from above, where we compared the two different ways of modelling a labelled transition system coalgebraically. Summing up, the first view (based on the input functor) gave us a system that responded to an input, while the second view (based on the output functor) generated output. It certainly is a legitimate approach to combine both these functors to obtain an input-output-machine.

Example 2.4.5 ((Moore) Machine Functor) Let A and B be arbitrary sets. The machine functor with inputs from A and outputs in B is the endofunctor $M: \text{Set} \rightarrow \text{Set}$ where $MX = B \times X^A$ for each set X and $Mf = \text{id}_B \times f^A$ for each function $f: X \rightarrow Y$.

As the name suggests, a coalgebra $c = \langle o, s \rangle: X \rightarrow B \times X^A$ of this functor captures exactly the transition structure of a *Moore machine* [Moo56]. Given a state $x \in X$ the tuple $c(x) = (o(x), s(x)) \in B \times X^A$ specifies an *output value* $o(x)$ of this state as well as a unique *successor state* $s(x)(a) \in X$ for every input $a \in A$. The only missing ingredient for a complete Moore machine is a distinct initial state, which we can of course simply specify in addition to the coalgebra. This is, however, common for the coalgebraic modelling – initial states are not inherent but need to be defined separately.

If we consider the special case where $B = 2$, a coalgebra $c: X \rightarrow 2 \times X^A$ is simply a *deterministic automaton (DA)*. For a state $x \in X$ the Boolean value $o(x)$ now determines whether it is a *final state* ($o(x) = 1$) or not ($o(x) = 0$). Note that we do not restrict the cardinality of the state space X so that in contrast to the common theory of *finite* automata we are also able to define and work with *infinite* ones which is important for the coalgebraic behavioral analysis.

In order to model *nondeterministic automata (NA)*, we can combine the machine functor where $B = 2$ with the powerset functor. Then NA are the coalgebras of the form $c = \langle o, s \rangle: X \rightarrow 2 \times (\mathcal{P}X)^A$. Again, for a state $x \in X$ the Boolean $o(x)$ determines whether it is final or not and the successor function $s(x): A \rightarrow \mathcal{P}X$ now assigns to each input action $a \in A$ a set $s(x)(a) \subseteq X$ of successor states.

By Lemma 2.4.4 we know that $2 \times (\mathcal{P}X)^A \cong \mathcal{P}1 \times \mathcal{P}(A \times X) \cong \mathcal{P}(A \times X + 1)$. Thus if we are able to define an endofunctor $_ + 1$ on Set , we could equivalently express nondeterministic automata as coalgebras $X \rightarrow \mathcal{P}(A \times X + 1)$.

Definition 2.4.6 (Termination Functor) Let A be a set. The *termination functor* $_ + A: \text{Set} \rightarrow \text{Set}$ maps each set X to the set $X + A$ and any function $f: X \rightarrow Y$ to

the function $f + \text{id}_A: X + A \rightarrow X + A$ which is defined as $f + \text{id}_A((x, 0)) = f(x)$ and $f + \text{id}_A((a, 1)) = a$ for every $x \in X$ and every $a \in A$.

A coalgebra $c: X \rightarrow X + A$ of this functor corresponds to a very restricted type of deterministic transition system. For a state $x \in X$ there can either be a transition to another state $y \in X$ (if $c(x) = (y, 0)$) or the system terminates at x with an output $a \in A$ (if $c(x) = (a, 1)$).

Coming back to nondeterministic automata, we now have indeed succeeded in modelling them as coalgebras $c: X \rightarrow \mathcal{P}(A \times X + \mathbb{1})$ for the endofunctor $\mathcal{P} \circ (_ + \mathbb{1}) \circ (A \times _)$ on Set . Each state $x \in X$ gets assigned a subset $c(x) \subseteq A \times X + \mathbb{1}$ and is final if and only if this subset contains the termination symbol $\checkmark \in \mathbb{1}$. The possible transitions from x are given by the pairs $(a, y) \in c(x)$.

We conclude our short survey of coalgebraic transition system models by a brief look at probabilistic systems. Using essentially the same ideas as above, we can see that a reactive system is a coalgebra $c: X \rightarrow (\mathcal{D}X)^A$ and if we need final states it is a coalgebra $c: X \rightarrow 2 \times (\mathcal{D}X)^A$. In Chapter 5 we will generalize this a bit further by considering a probabilistic Moore machine with outputs in $[0, 1]$, i.e., a coalgebra $c: X \rightarrow [0, 1] \times (\mathcal{D}X)^A$.

A generative probabilistic system is a coalgebra $X \rightarrow \mathcal{D}(A \times X)$ or if we want to have final states a coalgebra $X \rightarrow \mathcal{D}(A \times X + \mathbb{1})$. We will look at these systems in a more general setting in Chapter 4.

2.4.2 Final Coalgebra

The coalgebras of an endofunctor F and their morphisms constitute a category which we denote by $\text{CoAlg}(F)$. We will now study the final objects of this category – if they exist – and see that they give rise to a notion of behavior.

Definition 2.4.7 (Final Coalgebra) Let F be an endofunctor on a category \mathcal{C} . A *final F -coalgebra* is a coalgebra $z: Z \rightarrow FZ$ such that for any other F -coalgebra $a: A \rightarrow FA$ there is a unique coalgebra morphism from a to z . We denote this morphism and the underlying \mathcal{C} -arrow from A to Z by $\llbracket \cdot \rrbracket_a$ or sometimes simply by $\llbracket \cdot \rrbracket$ if a is clear from the context.

As usual for final objects, a final coalgebra need not exist but if it does it is unique up to isomorphism. A first trivial example for a final coalgebra is the identity function $\text{id}_{\mathbb{1}}: \mathbb{1} \rightarrow \mathbb{1}$ on the singleton set $\mathbb{1}$. It certainly is a coalgebra for the identity functor Id_{Set} on Set . Moreover, the singleton $\mathbb{1}$ is a final object in Set so for each set X there is a unique function $!_X: X \rightarrow \mathbb{1}$ given by $!_X(x) = \checkmark$. This function is a coalgebra homomorphism from *any* coalgebra $c: X \rightarrow X$ to $\text{id}_{\mathbb{1}}$ so we can define $\llbracket \cdot \rrbracket_c := !_X$.

Before looking at more examples of final coalgebras we provide an important non-example. The powerset functor of Example 2.3.11 has no final coalgebra. In order to see this, we cite a simple but useful result on final coalgebras.

Lemma 2.4.8 (Lambek’s Lemma [Lam68, Lemma 2.2]) Let F be an endofunctor on an arbitrary category. Any final coalgebra $z: Z \rightarrow FZ$ is an isomorphism.

The proof of this result is not very difficult and can be found e.g. in the cited paper. Of course, this result rules out the possibility of a final coalgebra for the powerset functor since this would imply the existence of a set X such that there is an isomorphism between X itself and its powerset $\mathcal{P}X$ which cannot exist because the cardinality of $\mathcal{P}X$ is strictly greater than that of X itself⁹. In contrast to that, the finite powerset functor \mathcal{P}_f has a final coalgebra [Wor05].

Behavior via Finality

Let us now come back to functors for which a final coalgebra exists and look at these final coalgebras more closely as it will help to understand their expressive power. First we consider the final coalgebra of the output functor (this is also studied in the literature [Rutoo, Example 9.4]).

Example 2.4.9 (Final Coalgebra for the Output Functor) We claim that a final coalgebra for the output functor $A \times _$ of Example 2.4.3 is given by the function $z = \langle h, t \rangle: A^\omega \rightarrow A \times A^\omega$ which maps an infinite word $w: \mathbb{N}_0 \rightarrow A$ to the tuple $(h(w), t(w))$. Here, $h(w) = w(0) \in A$ is the first letter of w (the *head*) and $t(w) \in A^\omega$ is the rest of the word w (the *tail*) interpreted again as infinite word. Formally it is defined as the function $t(w): \mathbb{N}_0 \rightarrow A, t(w)(n) = w(n+1)$.

Let us now show that this is correct. Given a coalgebra $c = \langle o, s \rangle: X \rightarrow A \times X$ we need to define a unique function $\llbracket \cdot \rrbracket_c: X \rightarrow A^\omega$ such that the following diagram commutes.

$$\begin{array}{ccc}
 X & \xrightarrow{\llbracket \cdot \rrbracket_c} & A^\omega \\
 c = \langle o, s \rangle \downarrow & & \downarrow z = \langle h, t \rangle \\
 A \times X & \xrightarrow{F\llbracket \cdot \rrbracket = \text{id}_A \times \llbracket \cdot \rrbracket_c} & A \times A^\omega
 \end{array}$$

⁹This is known as *Cantor’s theorem* and the original proof technique is called *Cantor’s diagonal argument*, named after the German mathematician Georg Cantor who proved it in 1892 [Can92]. A set-theoretic proof of it can be found in a paper by Ernst Zermelo [Zero8, 32. Satz von Cantor].

Commutativity of this diagram is equivalent to requiring the equality

$$\langle h, t \rangle \circ \llbracket \cdot \rrbracket_c = (\text{id}_A \times \llbracket \cdot \rrbracket_c) \circ \langle o, s \rangle$$

which can simply be rewritten as

$$\langle h \circ \llbracket \cdot \rrbracket_c, t \circ \llbracket \cdot \rrbracket_c \rangle = \langle o, \llbracket \cdot \rrbracket_c \circ s \rangle.$$

If we plug in an element $x \in X$ in this equation and use the above definition of h and t we obtain the definition

$$\llbracket x \rrbracket_c(0) = o(x) \quad \text{and} \quad \forall n \in \mathbb{N}_0 : \llbracket x \rrbracket_c(n+1) = \llbracket s(x) \rrbracket_c(n). \quad (2.4.1)$$

Thus the commutativity of the diagram has almost immediately provided us with a unique, sound and complete definition of the coalgebra homomorphism $\llbracket \cdot \rrbracket_c : X \rightarrow A^\omega$ for any coalgebra $c : X \rightarrow A \times X$. Therefore $z = \langle h, t \rangle$ is indeed a final coalgebra.

Based on this example let us analyze how a final coalgebra is related to the behavior of transition systems. As we have discussed before, a coalgebra $c = \langle o, s \rangle$ for the output functor is a deterministic transition system with state labels. The unique coalgebra homomorphism $\llbracket \cdot \rrbracket_c$ into the final coalgebra as defined in Equation (2.4.1) maps each state $x \in X$ to an infinite word that corresponds to the sequence of state labels that one can observe when the system runs forever. In other words, $\llbracket x \rrbracket_c$ is just the unique element of the set $\mathcal{L}^\omega(x)$ of infinite traces of the state x .

As another standard example we consider again the machine functor $M = B \times _^A$ from Example 2.4.5 and its final coalgebra [JSS15, Lemma 3].

Example 2.4.10 (Final Coalgebra for the Machine Functor) A final coalgebra for the machine functor $M = B \times _^A$ from Example 2.4.5 is given by the function

$$z = \langle o_z, s_z \rangle : B^{A^*} \rightarrow B \times (B^{A^*})^A$$

which maps any function $f : A^* \rightarrow B$ to the tuple $z(f) = (o_z(f), s_z(f))$. The output value $o_z(f)$ is the value of f on the empty word, i.e., $o_z(f) = f(\varepsilon)$ and the successor function $s_z(f) : A \rightarrow B^{A^*}$ assigns to each letter $a \in A$ the function $s_z(f)(a) : A^* \rightarrow B$. Its value on a word $w \in A^*$ is equal to the value of f on the word aw , formally $s_z(f) = \lambda a. \lambda w. f(aw)$.

For an arbitrary coalgebra $c = \langle o, s \rangle : X \rightarrow B \times X^A$ the unique homomorphism $\llbracket \cdot \rrbracket_c : X \rightarrow B^{A^*}$ into the final coalgebra is given by the functions $\llbracket x \rrbracket_c : A^* \rightarrow B$ for every $x \in X$ where

$$\llbracket x \rrbracket_c(\varepsilon) = o(x), \quad \forall a \in A. \forall w \in A^*. \llbracket x \rrbracket_c(aw) = \llbracket s(x) \rrbracket_c(w). \quad (2.4.2)$$

This definition can be obtained using the same technique as above in Example 2.4.9.

Again we aim at interpreting the homomorphism into the final coalgebra as behavior of the system which is a deterministic Moore machine. For each state $x \in X$ the function $\llbracket x \rrbracket_c: A^* \rightarrow B$ maps any finite word $w \in A^*$ to the value $\llbracket x \rrbracket_c(w) \in B$. This is just the state label of the unique state in the Moore machine that can be reached when starting at x and traversing the system following the transitions specified by the letters of the word w .

In the special case of deterministic automata ($B = 2$) both the final coalgebra and the homomorphism into it can be interpreted in formal language theory (for more details on this special case the interested reader is invited to look into Jan Rutten's paper "Automata and Coinduction (An Exercise in Coalgebra)" [Rut98]). Recall that a *formal language* over an alphabet A is nothing but a subset $L \subseteq A^*$. Given a letter $a \in A$ the *a-derivative* of a language $L \subseteq A^*$ is the language $L_a := \{w \in A^* \mid aw \in L\}$. Using these derivatives, we can turn the set $\mathcal{P}(A^*)$ of all languages over A into a coalgebra (an automaton) $\mathbf{l} = \langle o_l, s_l \rangle: \mathcal{P}(A^*) \rightarrow 2 \times \mathcal{P}(A^*)^A$. For any language $L \subseteq A^*$ we simply define $o_l(L) = 1$ if $\varepsilon \in L$ and $o_l(L) = 0$ else. Moreover, for each $a \in A$ we define $s_l(L)(a) = L_a$. If we recall from Lemma 2.4.4 that $\mathcal{P}(A^*) \cong 2^{A^*}$ we can see that this is exactly the same as the final coalgebra z defined in Example 2.4.10 (above). Moreover, for any deterministic automaton $c: X \rightarrow 2 \times X^A$ the unique coalgebra homomorphism $\llbracket \cdot \rrbracket_c: X \rightarrow 2^{A^*}$ maps each state $x \in X$ to the language $\llbracket x \rrbracket_c: A^* \rightarrow 2$ it accepts.

Based on our observations in these two examples, we now formally define behavioral equivalence for Set functors.

Definition 2.4.11 (Behavioral Equivalence for Set-Functors) Let F be an endofunctor on **Set** for which a final coalgebra $z: Z \rightarrow FZ$ exists. For any coalgebra $\alpha: A \rightarrow FA$ we define two states $x, y \in A$ to be *behaviorally equivalent* if they are mapped to the same state in the final coalgebra, i.e., if $\llbracket x \rrbracket_\alpha = \llbracket y \rrbracket_\alpha$.

This definition can easily be adapted for categories which are similar to **Set** in the sense that their objects are essentially sets with structure and their arrows are functions with structure. Examples of such a category include the category of measurable spaces and measurable functions, **Meas**, which we will encounter in Chapter 4, the category of pseudometric spaces and nonexpansive functions, **PMet**, which we will discuss in details in Chapter 5 and of course also Kleisli-categories of **Set**-monads.

Moreover, in Chapter 3 we will discuss an alternative approach by considering

behavioral equivalences between arrows instead of states of a system.

Final Coalgebra and Bisimilarity

Let us now discuss what type of behavior is captured by the above definition. Based on the examples we have considered so far, we might be tempted to think that it is trace equivalence. However, this is a misleading thought. So far, all the examples for which we looked at a final coalgebra were *deterministic* systems for which trace equivalence and bisimilarity coincide. We will now show that the unique map into the final coalgebra usually characterizes the equivalence classes of a coalgebraic version of bisimilarity.

Definition 2.4.12 (Bisimulation for Set-functors [AM89]) Let F be an endofunctor on Set and $c: X \rightarrow FX$ be a coalgebra. A relation $R \subseteq X \times X$ is called an F -bisimulation on c if there is a coalgebra $r: R \rightarrow FR$ such that the projections $\pi_1, \pi_2: R \rightarrow X$ (which are the restrictions of the binary product projections to R) are coalgebra homomorphisms, i.e., such that the following diagram commutes.

$$\begin{array}{ccccc}
 X & \xleftarrow{\pi_1} & R & \xrightarrow{\pi_2} & X \\
 c \downarrow & & \downarrow r & & \downarrow c \\
 FX & \xleftarrow{F\pi_1} & FR & \xrightarrow{F\pi_2} & FX
 \end{array}$$

Similarly, an F -bisimulation between two coalgebras $c_1: X_1 \rightarrow FX_1$, $c_2: X_2 \rightarrow FX_2$ is a relation $R \subseteq X_1 \times X_2$ with a coalgebraic structure $r: R \rightarrow FR$ satisfying $c_i \circ \pi_i = F\pi_i \circ c_i$.

One can show [Rutoo, Corollary 5.6] that the union of all F -bisimulations on a coalgebra $c: X \rightarrow FX$ is again an F -bisimulation and moreover an equivalence relation. As for the usual notion of bisimulation, we will call it F -bisimilarity and denote it by \sim_c or simply by \sim .

The coalgebraic notion of F -bisimulation encompasses the original definition of bisimulation if we instantiate it to the two Set -functors that we use to model LTS. We will show this for the coalgebras of the Set -functor $(\mathcal{P}_-)^A$. In the literature this is usually described for the alternative model of an LTS as coalgebra $c: X \rightarrow \mathcal{P}(A \times X)$ [RT93, Example 2.3], [Rutoo, Example 2.1 (continued)].

Example 2.4.13 (LTS Bisimulation as Coalgebraic Bisimulation) For a coalgebra $c: X \rightarrow (\mathcal{P}X)^A$ we have a transition $x \xrightarrow{a} x'$ if and only if $x' \in c(x)(a)$.

Using this notation, a bisimulation in the sense of Definition 2.2.4 is a binary relation $R \subseteq X \times X$ such that for every $(x_1, x_2) \in R$ and every $a \in A$ we have that

- ▷ for every $x'_1 \in c(x_1)(a)$ there is an $x'_2 \in c(x_2)(a)$ with $(x'_1, x'_2) \in R$, and
- ▷ for every $x'_2 \in c(x_2)(a)$ there is an $x'_1 \in c(x_1)(a)$ with $(x'_1, x'_2) \in R$.

Given any such relation we get a new coalgebra $r: R \rightarrow (\mathcal{P}R)^A$ by defining

$$r(x_1, x_2)(a) := \{(x'_1, x'_2) \in R \mid x'_1 \in c(x_1)(a) \wedge x'_2 \in c(x_2)(a)\}$$

for every $x_1, x_2 \in X$ and every $a \in A$. Commutativity of the diagram

$$\begin{array}{ccccc} X & \xleftarrow{\pi_1} & R & \xrightarrow{\pi_2} & X \\ c \downarrow & & \downarrow r & & \downarrow c \\ (\mathcal{P}X)^A & \xleftarrow{(\pi_1[\cdot])^A} & (\mathcal{P}R)^A & \xrightarrow{(\pi_2[\cdot])^A} & (\mathcal{P}X)^A \end{array}$$

is equivalent to the requirement that for all $(x_1, x_2) \in R$ and all $a \in A$ and $i \in \{1, 2\}$ the equality $c(x_i)(a) = \pi_i[r(x_1, x_2)(a)]$ holds. We calculate

$$\pi_i[r(x_1, x_2)(a)] = \{x'_i \in X \mid (x'_1, x'_2) \in R \wedge x'_1 \in c(x_1)(a) \wedge x'_2 \in c(x_2)(a)\}$$

and using the fact that R is a bisimulation and $(x_1, x_2) \in R$ we easily see that this is indeed equal to $c(x_i)(a)$.

Conversely let $R \subseteq X \times X$ be an F -bisimulation with transition structure $r: R \rightarrow (\mathcal{P}R)^A$ such that the diagram commutes. Now let $(x_1, x_2) \in R$ and $a \in A$. By commutativity of the diagram we know that $c(x_1)(a) = \pi_1[r(x_1, x_2)(a)]$ so for any $x'_1 \in c(x_1)(a)$ there is a pair $(x'_1, x'_2) \in r(x_1, x_2)(a) \subseteq R$ and moreover $x'_2 \in \pi_2[r(x_1, x_2)(a)] = c(x_2)(a)$. This works analogously to show the other implication so we conclude that R is a bisimulation in the classical sense.

Now that we have seen that the coalgebraic definition of F -bisimulation coincides with the classical notion for LTS, we compare it with the unique map into the final coalgebra. One property is very easy to show.

Theorem 2.4.14 ([RT93, Theorem 2.5]) Let F be an endofunctor on \mathbf{Set} for which a final coalgebra $z: Z \rightarrow FZ$ exists and $c: X \rightarrow FX$ be an arbitrary coalgebra. Moreover, let $\llbracket \cdot \rrbracket_c: c \rightarrow z$ be the unique arrow into the final coalgebra. For all $x, x' \in X$ we have

$$x \sim_c x' \implies \llbracket x \rrbracket_c = \llbracket x' \rrbracket_c.$$

In order to also obtain the converse of the above implication it is sufficient to require that the functor preserves weak pullbacks.

Theorem 2.4.15 ([Rutoo, Theorem 9.3]) Let F be an endofunctor on \mathbf{Set} for which a final coalgebra $z: Z \rightarrow FZ$ exists and $c: X \rightarrow FX$ be an arbitrary coalgebra. If F preserves weak pullbacks we have for all $x, x' \in X$ that

$$x \sim_c x' \iff \llbracket x \rrbracket_c = \llbracket x' \rrbracket_c.$$

Thus $\llbracket x \rrbracket_c$ represents the \sim_c -equivalence class of x .

Let us now interpret this result for labelled transition systems. First of all, it is not applicable to all LTS, since both coalgebraic models we have seen involve the general powerset functor, so neither of them has a final coalgebra. However, this *technical problem* can be remedied by considering only *finitely branching* LTS which can be modelled by replacing the powerset functor \mathcal{P} with its finite variant \mathcal{P}_f .

The second conclusion we can draw from the result is that the coalgebraic behavioral equivalence as defined in Definition 2.4.11 is not suitable to obtain trace semantics for nondeterministic systems because for them bisimulation is strictly finer than trace equivalence.

2.4.3 Trace Semantics

In light of our previous observations we now look for a coalgebraic method to obtain trace semantics. This search has turned out to be a challenge for the coalgebraic community and while several approaches have been suggested in the past, this is still an area of active research (see e.g. [SBBR13; KMPS15; JSS15; MPS15; UH15; KR15]) during the writing of this thesis.

Here, we will focus on two conceptually simple approaches that fit nicely into the categorical framework and are the ones employed in the main parts of this thesis. Both share the common prerequisite that the functor whose coalgebras are to be considered allows a decomposition into an endofunctor and a monad functor. However, there are two possible decompositions, namely

$$c: X \rightarrow TFX, \quad \text{or} \quad (2.4.3)$$

$$c: X \rightarrow FTX \quad (2.4.4)$$

where T is the endofunctor of a monad (T, η, μ) and F is an arbitrary endofunctor on a common category \mathcal{C} . The idea is that the monad models a side-effect, like nondeterminism or probabilistic branching, whereas F models the explicit branching of the system.

We have already come across examples for both of these variants. First of all, we have seen that nondeterministic automata are coalgebras of the form $X \rightarrow 2 \times (\mathcal{P}X)^A$ which is indeed of the latter type by taking as monad the powerset monad of Example 2.3.35 and as endofunctor the machine functor $2 \times _{}^A$ of Example 2.4.5 with output set $B = 2$. Alternatively, we have modelled NA as coalgebras $X \rightarrow \mathcal{P}(A \times X + \mathbb{1})$ which – using the same monad and the endofunctor $F = A \times _{} + \mathbb{1}$ – clearly is of the first type.

If we substitute the powerset monad by the distribution monad of Example 2.3.36 in the examples above, we conclude that generative probabilistic systems fit into the first approach and reactive ones into the second.

Traces in the Kleisli Category

Let us now examine the first approach to trace semantics for TF-coalgebras as in Equation (2.4.3) which is based on initial work by John Power and Daniele Turi [PT99] and has more recently been promoted and extended by Ichiro Hasuo, Bart Jacobs and Ana Sokolova [HJS06; HJS07] and which we will employ in Chapter 4.

If we have a Kleisli-law $\lambda: FT \Rightarrow TF$ as defined in Definition 2.3.43 we can by Theorem 2.3.44 define an extension $\hat{F}: \mathcal{Kl}(T) \rightarrow \mathcal{Kl}(T)$ of the endofunctor F to the Kleisli-category of the monad.

By definition of the arrows in a Kleisli-category, a TF-coalgebra $c: X \rightarrow TFX$ can equivalently be seen as an \hat{F} -coalgebra $c: X \rightsquigarrow \hat{F}X$ in $\mathcal{Kl}(T)$. If there is a final \hat{F} -coalgebra we can now define trace semantics for our TF-coalgebra using the unique arrow into the final coalgebra.

Definition 2.4.16 (Trace Semantics in the Kleisli Category) Let (T, η, μ) be a monad and F be an endofunctor on a common category \mathcal{C} and $\hat{F}: \mathcal{Kl}(T) \rightarrow \mathcal{Kl}(T)$ be an extension of F . Suppose that a final \hat{F} -coalgebra $z: Z \rightarrow T\hat{F}Z$ exists. For any TF-coalgebra $c: X \rightarrow TFX$ we define its *trace semantics* $\text{tr}_c: X \rightarrow TZ$ to be the unique \mathcal{C} -arrow underlying the final coalgebra homomorphism $\llbracket \cdot \rrbracket_c: X \rightsquigarrow Z$.

One important thing to notice about this definition is that the side effects specified via the monad (nondeterminism, probability) are now contained in the unique map $\llbracket \cdot \rrbracket_c: X \rightsquigarrow Z$ into the final coalgebra which corresponds to an arrow $\llbracket \cdot \rrbracket_c: X \rightarrow TZ$.

In order to apply the above definition we need to have a final coalgebra for the lifted functor. The main contribution of [HJS06] is that in Set this final coalgebra arises from an initial algebra provided that the monad has a suitable order structure [HJS06, Theorem 3].

Since both the powerset monad and the subdistribution monad (but not the distribution monad) satisfy these assumptions, we can obtain both the traces of arbitrary LTS and discrete generative probabilistic systems as given in Equations (2.2.4) to (2.2.6).

As said in the beginning, we will employ this approach to trace semantics in Chapter 4 but we will not be able to use the main result of [HJS06]. The reason for this is that we will work in a category other than \mathbf{Set} . Thus we will just use the above definition of trace equivalence and define the necessary final coalgebra by hand.

Traces via the Generalized Powerset Construction

Now we look at the second approach for FT-coalgebras as in Equation (2.4.4) which is based on a coalgebraic view on determinization of nondeterministic automata via the powerset construction [Rutoo, Exercise 15.4]. It has been systematically studied by Alexandra Silva, Filippo Bonchi, Marcello Bonsangue and Jan Rutten as the *generalized powerset construction* [SBBR10; SBBR13]. Later Bart Jacobs, Alexandra Silva and Ana Sokolova demonstrated that it can also be extended to encompass the first approach presented above [JSS12; JSS15]. We will follow their presentation of how to obtain trace semantics via the generalized powerset construction.

In presence of an \mathcal{EM} -law $\lambda: TF \Rightarrow FT$ we can construct an F-coalgebra based on an FT-coalgebra $c: X \rightarrow FTX$ by defining

$$c^\sharp := \left(TX \xrightarrow{Tc} TFTX \xrightarrow{\lambda_{TX}} FTTX \xrightarrow{F\mu_X} FTX \right).$$

We can interpret this to be the coalgebraic *determinization* of the original system. The side effect that is specified by the monad now is not any longer part of the transition structure $X \rightarrow FTX$ but part of the new state space TX . Indeed, this object is equipped with the free algebra structure $\mu_X: TTX \rightarrow TX$.

Under the hood, the transformation of c into c^\sharp corresponds to applying a functor L to c which is a *lifting* of the free algebra functor $L^T: \mathcal{C} \rightarrow \mathcal{EM}(T)$ as given in Definition 2.3.41 in the sense that it makes the diagram in Figure 2.4.1 commute [JSS15, Lemma 1]. In that diagram \mathcal{C} is the category on which both the endofunctor F and the monad (T, η, μ) are defined, U and U' are the forgetful functors mapping a coalgebra to its carrier and a coalgebra homomorphism to the underlying arrow and \hat{F} is the unique lifting of F to the Eilenberg-Moore category that arises from the \mathcal{EM} -law λ by Theorem 2.3.44. The coalgebra c^\sharp as defined above is the function underlying the \hat{F} -coalgebra $Lc: \mu_X \rightarrow \hat{F}\mu_X$

whose carrier is the free T -algebra μ_X on X , i.e., $c^\sharp = U^T Lc: TX \rightarrow FTX$ where $U^T: \mathcal{EM}(T) \rightarrow \mathcal{C}$ is the forgetful functor mapping an algebra to its carrier.

$$\begin{array}{ccc}
 \text{CoAlg}(FT) & \xrightarrow{L} & \text{CoAlg}(\widehat{F}) \\
 \downarrow U & & \downarrow U' \\
 \mathcal{C} & \xrightarrow{L^T} & \mathcal{EM}(T)
 \end{array}$$

Figure 2.4.1: Lifting of the free algebra functor

If we now consider the category of \widehat{F} -coalgebras more carefully, we can see that the \mathcal{EM} -law permits to lift final F -coalgebras to final \widehat{F} -coalgebras.

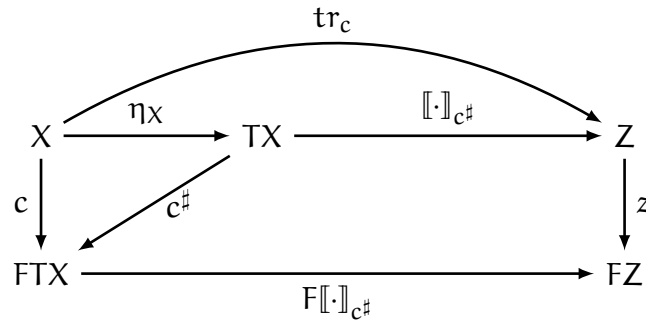
Theorem 2.4.17 (Final Coalgebra Lifting [JSS15, Prop. 3]) Let (T, η, μ) be a monad and F be an endofunctor on a common category \mathcal{C} and $\lambda: TF \Rightarrow FT$ an \mathcal{EM} -law. If F has a final coalgebra $z: Z \rightarrow FZ$ in \mathcal{C} then Z carries a T -algebra structure $\alpha: TZ \rightarrow Z$ obtained by finality as depicted in the diagram below.

$$\begin{array}{ccc}
 TZ & \xrightarrow{\alpha} & Z \\
 \lambda \circ Tz \downarrow & & \downarrow z \\
 TFZ & \xrightarrow{F\alpha} & FZ
 \end{array}$$

Moreover, z is a homomorphism of algebras $z: \alpha \rightarrow \widehat{F}\alpha$ which is the final coalgebra for the lifted functor $\widehat{F}: \mathcal{EM}(T) \rightarrow \mathcal{EM}(T)$.

If a final F -coalgebra $z: Z \rightarrow FZ$ exists one can thus define a semantic map for the FT -coalgebra c into Z as follows.

Definition 2.4.18 (Trace Semantics via the Generalized Powerset Construction) Let (T, η, μ) be a monad and F be an endofunctor on a common category \mathcal{C} and $\widehat{F}: \mathcal{EM}(T) \rightarrow \mathcal{EM}(T)$ be a lifting of F . Suppose that a final F -coalgebra $z: Z \rightarrow FZ$ exists. For any FT -coalgebra $c: X \rightarrow FTX$ we define its *trace semantics* to be $\text{tr}_c := \llbracket \cdot \rrbracket_{c^\sharp} \circ \eta_X: X \rightarrow Z$. The situation is summarized in the following diagram.



This definition amounts to carrying out the following steps (see [JSS15, Definition 1]) for a given coalgebra $c: X \rightarrow FTX$.

1. First we *determinize* the system by applying L to obtain the F -coalgebra $c^\# = U^T Lc$.
2. In the determinized system we can determine the behavioral equivalence via finality, i.e., we consider the coalgebra map $[[\cdot]]_{c^\#}$.
3. In order to obtain the behavior of the original system, we embed it into its determinization via the unit to obtain its trace semantics as $[[\cdot]]_{c^\#} \circ \eta_X$.

We will employ this approach in the end of Chapter 5. Let us now quickly illustrate it for the example of nondeterministic automata as already mentioned in the beginning [Rutoo, Exercise 15.4].

For this example, the base category \mathcal{C} is \mathbf{Set} , the functor F is the deterministic automaton functor $2 \times _^A$ and the monad is the powerset monad (\mathcal{P}, η, μ) of Example 2.3.35. As \mathcal{EM} -law we use the following.

Definition 2.4.19 (\mathcal{EM} -law for Nondeterministic Automata [JSS15, p. 867])

Let (\mathcal{P}, η, μ) be the powerset monad from Example 2.3.35 and $F = 2 \times _^A$ be the deterministic machine functor. The \mathcal{EM} -law $\lambda: \mathcal{P}(2 \times _^A) \Rightarrow 2 \times \mathcal{P}(_)^A$ is defined, for any set X , as $\lambda_X = \langle o, s \rangle$ with $o(S) = 1$ if there is an $s' \in X^A$ such that $(1, s') \in S$ else $o(S) = 0$ and the successor functions

$$s(S): A \rightarrow \mathcal{P}X, \quad s(A) = \{s'(a) \mid (o', s') \in S\}$$

for every $S \in \mathcal{P}(2 \times X^A)$

Using the final coalgebra $z: A^* \rightarrow \mathcal{P}(A^*)$ of the machine functor as in Example 2.4.10 the diagram of Definition 2.4.18 turns into the diagram in Figure 2.4.2 for a given nondeterministic automaton $c: X \rightarrow 2 \times (\mathcal{P}X)^A$. Let us now carry out the steps from above.

1. The determinization of the system by applying L yields the $\widehat{2 \times _^A}$ -coalgebra

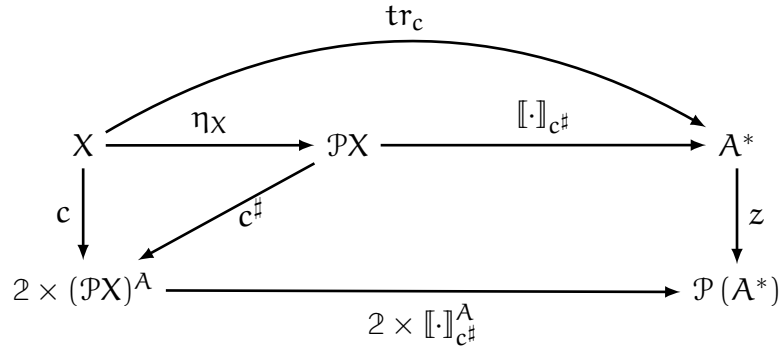


Figure 2.4.2: Usual trace semantics for nondeterministic automata via the generalized powerset construction

- $c^\sharp = U^T Lc$ which is just the usual powerset automaton. Thus for $c = \langle o, s \rangle$ we have $c^\sharp = \langle o^\sharp, s^\sharp \rangle$. For a set $S \subseteq X$ of states of the original automaton is final ($o^\sharp(S) = 1$) if and only if there is a final state $x \in S$, i.e., a state with $o(x) = 1$. Moreover, the unique a -successor of that set of states is the union of all a -successors of the states $x \in S$, i.e., the function $s^\sharp(S): A \rightarrow PX$ given by the assignment $s^\sharp(S)(a) = \{s(x)(a) \mid x \in S\}$.
2. Since the powerset automaton is a deterministic automaton, the behavioral equivalence induced via finality is simultaneously bisimilarity and language equivalence. The final coalgebra map $[\![\cdot]\!]_{c^\sharp}: PX \rightarrow A^*$ maps a state of the powerset automaton c^\sharp (i.e., a set of states of the original one) to the language it accepts.
 3. The behavior of a state $x \in X$ of the original automaton c is now given by considering the language of the corresponding singleton $\{x\}$. This is achieved by precomposing the semantic map $[\![\cdot]\!]_{c^\sharp}$ with the unit η_X of the powerset monad which maps each element to the corresponding singleton.

Adjunctions and Automata

WHEN studying coalgebras in various categories a natural question to ask is how to transform such coalgebras from one representation into another. Our motivating examples come from the world of deterministic and nondeterministic automata where various forms of determinization can be seen as functors which map coalgebras living in one category, into coalgebras living in another category. For instance, nondeterministic automata living in \mathbf{Rel} can be transformed into deterministic automata in \mathbf{Set} via the powerset construction. In the other direction, a deterministic automaton in \mathbf{Set} can be trivially regarded as a nondeterministic automaton in \mathbf{Rel} . It turns out that the transformations together form an adjunction between categories of coalgebras where the powerset construction is the right adjoint. In the same vein various other determinization-like constructions arise as adjunctions.

In the following we will first show under which circumstances an adjunction between two categories can be lifted to an adjunction between categories of coalgebras. Part of the answer was already given by Claudio Hermida and Bart Jacobs [HJ98] and we extend their characterization by giving another, equivalent, condition. Then we study several examples in detail, especially various forms of automata. Apart from the well-known deterministic and nondeterministic automata, we consider codeterministic (or backwards-deterministic) automata which arise during the application of Brzozowski’s minimization algorithm and have been studied in more details as *átomata* [BT11]. Moreover, we look at deterministic join automata, which are automata that have an algebraic structure on the states, allowing to take the join of a given set of states. Such automata live in the category \mathbf{JSL} of join semilattices, which is the Eilenberg-Moore category of the powerset monad on \mathbf{Set} (whereas \mathbf{Rel} is the Kleisli category of the powerset monad) and have already been considered in [SBBR13]. In total we consider four different adjunctions between such automata.

In order to explain what these adjunctions really mean in terms of behavioral equivalence, we study a general notion of behavioral equivalence for arbitrary categories. We first observe that the final coalgebra, if it exists, is preserved by right adjoints and hence can be “inherited” from coalgebras living in a different

category. Furthermore we show how queries on behavioral equivalence can be translated to equivalent queries on coalgebras in another category. This reflects the well-known construction of determinizing a nondeterministic automaton before answering questions about language equivalence.

Additional proofs and calculations for the provided results can be found in Appendix A.1.

3.1 Lifting Adjunctions

Within this section we are first going to present a short, motivating example which introduces our approach. Based on this, we then start to develop our lifting theory which yields our main theoretical result (Theorem 3.1.2). The result itself is not too surprising and, in fact, was discovered already earlier by Claudio Hermida and Bart Jacobs [HJ98] in a different setting (we will compare our approach with their result) and can be obtained using standard (2-)categorical methods [KS74]. However, the focus of our work is *not just the theory itself* but we are more interested in *how this theory helps to understand* certain (algorithmic) constructions on automata by *applying* it to various types of automata, modeled as coalgebras.

3.1.1 Motivating Example

Consider the (non-commutative) diagram of functors in Figure 3.1.1 where the bottom part is the canonical Kleisli adjunction as given in Definition 2.3.38 between \mathbf{Set} and \mathbf{Rel} . Let A be an alphabet, i.e., a finite set of labels. We

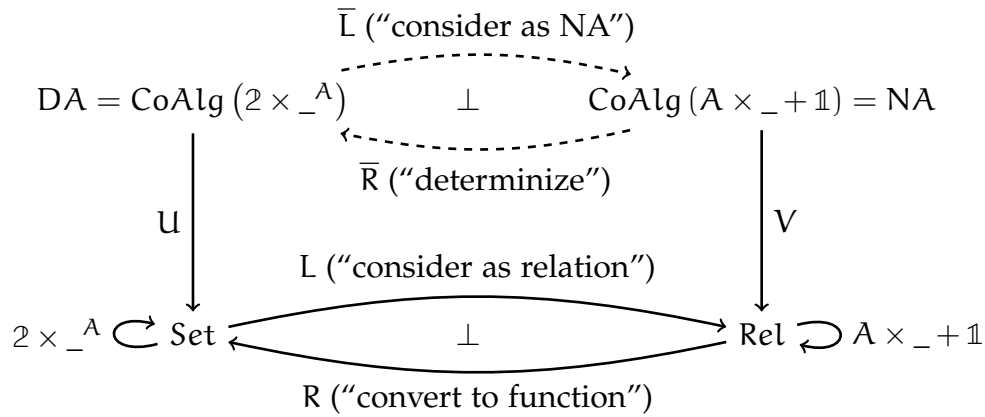


Figure 3.1.1: Lifting of the Kleisli adjunction

have already seen in Section 2.4.1 that the coalgebras for the functor $2 \times _ ^A$ on

Set are the deterministic automata. (DA). Moreover, using the fact that the Kleisli category of the powerset monad is isomorphic to \mathbf{Rel} , nondeterministic automata (NA) are coalgebras for a functor $A \times _ + \mathbb{1}$ on \mathbf{Rel} (we will discuss this more thoroughly later in Section 3.2.1). We aim at finding the functors \bar{L}, \bar{R} (dashed arrows on top) that form an adjunction which is a *lifting* of the original adjunction and we will see that for this particular example everything works out as planned and the lifted right adjoint \bar{R} “performs” the well-known powerset construction to determinize an NA.

3.1.2 Lifting an Adjunction to Coalgebras

The coalgebraic treatment of automata has provided several new views on algorithms for minimization and (co)determinization [ABH+12; BBRs12; BKP12; SBBR13; JSS15]. In all these publications the authors make use of certain adjunctions of categories to obtain the minimization or determinization of (various kinds of) automata.

We shall hereafter try to find and analyze a common and generic pattern on how we can make use of an adjunction $(L \dashv R, \eta, \epsilon) : \mathcal{C} \rightarrow \mathcal{D}$ to reason about and to find constructions (algorithms) on automata modeled as coalgebras. For that purpose let us fix two endofunctors $F : \mathcal{C} \rightarrow \mathcal{C}$ and $G : \mathcal{D} \rightarrow \mathcal{D}$ and look at the (non-commutative) diagram of functors in Figure 3.1.2 where $U : \mathbf{CoAlg}(F) \rightarrow \mathcal{C}$ and $V : \mathbf{CoAlg}(G) \rightarrow \mathcal{D}$ are the forgetful functors mapping a coalgebra to its carrier and a coalgebra homomorphism to the underlying arrow. The question

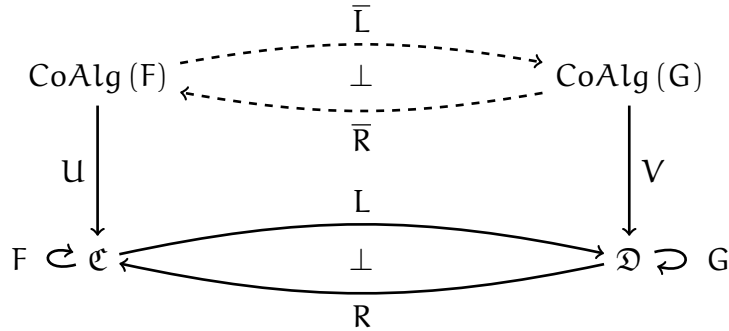


Figure 3.1.2: Lifting an adjunction to coalgebras

we are interested in is whether we can in some canonical way obtain the functors \bar{L} and \bar{R} as indicated by the dashed lines such that they form an adjunction which “arises” from the initial adjunction. A precise definition for this is given below. In several cases such adjoint functors transform coalgebras in a way that

we (re)discover algorithmic constructions on the modeled automata and we will back this hypothesis by the examples given in the following sections.

Definition 3.1.1 (Lifting) Let \mathcal{C} and \mathcal{D} be categories, $F: \mathcal{C} \rightarrow \mathcal{C}$, $G: \mathcal{D} \rightarrow \mathcal{D}$ be endofunctors and $U: \text{CoAlg}(F) \rightarrow \mathcal{C}$ and $V: \text{CoAlg}(G) \rightarrow \mathcal{D}$ be the forgetful functors mapping a coalgebra to its carrier and a coalgebra morphism to the underlying arrow. Let $(L \dashv R, \eta, \varepsilon): \mathcal{C} \rightarrow \mathcal{D}$ be an adjunction.

1. We call a functor $\bar{L}: \text{CoAlg}(F) \rightarrow \text{CoAlg}(G)$ [$\bar{R}: \text{CoAlg}(G) \rightarrow \text{CoAlg}(F)$] a *lifting* of L [R] if it satisfies the equality $V\bar{L} = L U$ [$U\bar{R} = R V$].
2. We call an adjunction $(\bar{L} \dashv \bar{R}, \bar{\eta}, \bar{\varepsilon}): \text{CoAlg}(F) \rightarrow \text{CoAlg}(G)$ a *lifting* of the adjunction $(L \dashv R, \eta, \varepsilon): \mathcal{C} \rightarrow \mathcal{D}$ if \bar{L} is a lifting of L , \bar{R} is a lifting of R and we have $U\bar{\eta} = \eta$ and $V\bar{\varepsilon} = \varepsilon$.

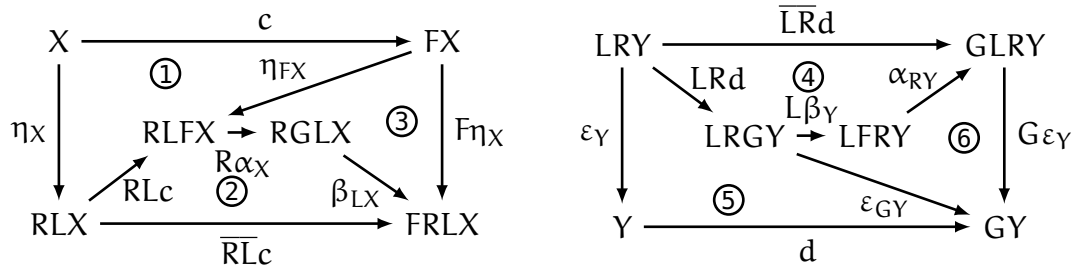
Although this definition is straightforward it has one setback: it does not tell us how to construct a lifted adjunction. Let us therefore introduce a method for handling this. If we had a natural transformation $\alpha: LF \Rightarrow GL$ it is not hard to see that we obtain a functor $\bar{L}: \text{CoAlg}(F) \rightarrow \text{CoAlg}(G)$ by defining

$$\bar{L}(X \xrightarrow{c} FX) = (LX \xrightarrow{Lc} LFX \xrightarrow{\alpha_X} GLX), \quad \bar{L}f = Lf \quad (3.1.1)$$

for all F -coalgebras $c: X \rightarrow FX$ and all F -coalgebra homomorphisms f and analogously, given a natural transformation $\beta: RG \Rightarrow FR$ we can define a functor $\bar{R}: \text{CoAlg}(G) \rightarrow \text{CoAlg}(F)$ by

$$\bar{R}(Y \xrightarrow{d} GY) = (RY \xrightarrow{Rd} RGY \xrightarrow{\beta_Y} FRY), \quad \bar{R}g = Rg \quad (3.1.2)$$

for all G -coalgebras $d: Y \rightarrow GY$ and all G -coalgebra homomorphisms g . By definition these functors are liftings and thus the only remaining question is whether we obtain a lifting of the adjunction. The equation $U\bar{\eta} = \eta$ can be spelled out as the requirement that for all F -coalgebras $c: X \rightarrow FX$ the arrow $\eta_X: X \rightarrow RLX$ is an F -coalgebra homomorphism $c \rightarrow \bar{R}\bar{L}c$ and likewise the equation $V\bar{\varepsilon} = \varepsilon$ translates to the requirement that for every G -coalgebra $d: Y \rightarrow GY$ the arrow $\varepsilon_Y: LRY \rightarrow Y$ is a G -coalgebra homomorphism $\bar{L}\bar{R}d \rightarrow d$. This is the case if and only if the outer rectangles of the following two diagrams commute.



These diagrams certainly commute if their inner parts commute: ① commutes because η is a natural transformation, ② by definition of $\overline{R}Lc$ and commutativity of ③ is equivalent to $F\eta_X = \beta_{LX} \circ R\alpha_X \circ \eta_{FX}$. Moreover, ④ commutes by definition of $\overline{L}Rd$ and ⑤ because ε is a natural transformation. Finally, the commutativity of ⑥ is equivalent to $\varepsilon_{GY} = G\varepsilon_Y \circ \alpha_{RY} \circ L\beta_Y$.

With these observations at hand it is easy to spell out a sufficient condition for the existence of a lifting which we will do in the following theorem.

Theorem 3.1.2 (Lifting an Adjunction to Coalgebras) Let \mathcal{C}, \mathcal{D} be categories, $F: \mathcal{C} \rightarrow \mathcal{C}$ and $G: \mathcal{D} \rightarrow \mathcal{D}$ be endofunctors and $(L \dashv R, \eta, \varepsilon): \mathcal{C} \rightarrow \mathcal{D}$ be an adjunction. There is a lifting $(\overline{L} \dashv \overline{R}, \overline{\eta}, \overline{\varepsilon}): \text{CoAlg}(F) \rightarrow \text{CoAlg}(G)$ of the adjunction if one of the following two equivalent conditions is fulfilled.

1. There are two natural transformations $\alpha: LF \Rightarrow GL$ and $\beta: RG \Rightarrow FR$ satisfying the following equalities.

$$F\eta = \beta L \circ R\alpha \circ \eta F \quad (3.1.3)$$

$$\varepsilon G = G\varepsilon \circ \alpha R \circ L\beta \quad (3.1.4)$$

2. There is a natural isomorphism $\beta: RG \Rightarrow FR$. [HJ98, 2.15 Corollary]

If 1 holds, the *adjoint mate* α^\bullet of α , which is defined as

$$\alpha^\bullet := RG\varepsilon \circ R\alpha R \circ \eta FR \quad (3.1.5)$$

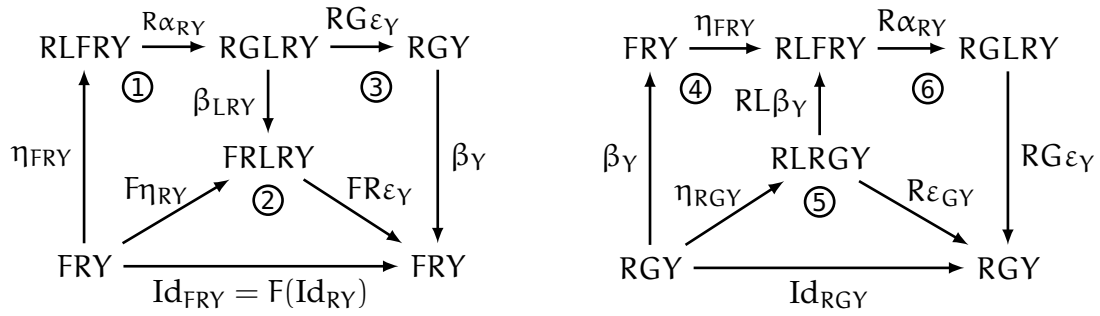
is the inverse of β . Conversely, if 2 holds we can define α as the adjoint mate $(\beta^{-1})^\bullet$ of β^{-1} which is defined as

$$(\beta^{-1})^\bullet = \varepsilon GL \circ L\beta^{-1}L \circ LF\eta. \quad (3.1.6)$$

In both cases \overline{L} and \overline{R} are defined by (3.1.1) and (3.1.2).

Proof. By the observations from above it should be quite clear, that (1) is sufficient for a lifting to exist. The fact that the second condition (2) of this theorem is also sufficient for the existence of a lifting is due to a result by Claudio Hermida and Bart Jacobs [HJ98, 2.15 Corollary]. They derive this as a by-product from a quite generic result in 2-categories using the fact that coalgebras are certain inserters in the 2-category of categories, functors and natural transformations. Thus in order to prove the theorem we just have to show that (1) and (2) are equivalent using the provided definitions of β^{-1} (3.1.5) and α (3.1.6).

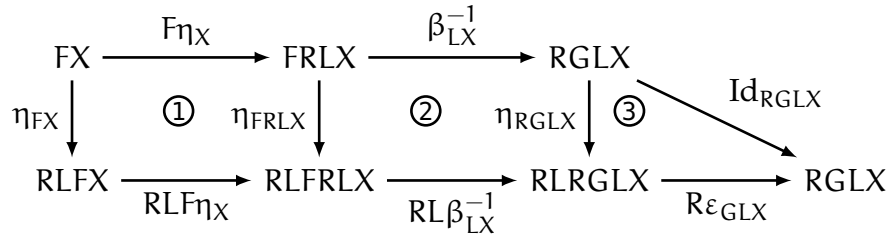
(1) \Rightarrow (2): The equations $\beta_Y \circ \alpha_Y^\bullet = \text{Id}_{FRY}$ and $\alpha_Y^\bullet \circ \beta_Y = \text{Id}_{RGY}$ are equivalent to commutativity of the outer rectangles of the following diagrams.



The diagrams commute because their inner parts commute: For the left diagram ① is (3.1.3) applied to $X = RY$, ② is F applied to the second unit-counit equation (2.3.3) and ③ is the natural transformation diagram for β . For the right diagram we observe that ④ is the natural transformation diagram for η , ⑤ is the second unit-counit equation (2.3.3) applied to GY and ⑥ is R applied to (3.1.4). Thus β is indeed a natural isomorphism with inverse α^\bullet .

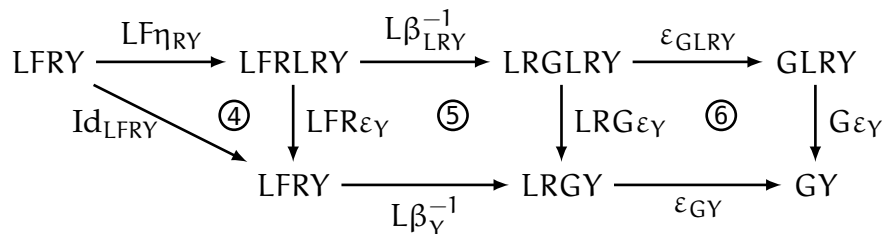
(2) \Rightarrow (1): We have to show that α defined by (3.1.6) satisfies (3.1.3) and (3.1.4).

We first show (3.1.3): Let X be an arbitrary \mathfrak{C} -object. Then $F\eta_X = \beta_{LX} \circ R\alpha_X \circ \eta_{FX}$ holds if and only if $\beta_{LX}^{-1} \circ F\eta_X = R\epsilon_{GLX} \circ RL\beta_{LX}^{-1} \circ RL\eta_X \circ \eta_{FX}$ holds which in turn is equivalent to commutativity of the outer part of the following diagram.



① and ② commute because η is a natural transformation from $Id_{\mathfrak{C}}$ to RL , functors preserve inverses and ③ is the second unit-counit equation (2.3.3) applied to GLX .

Now we show (3.1.4): If Y is an arbitrary \mathfrak{D} -object $\epsilon_{GY} = G\epsilon_Y \circ \alpha_{RY} \circ L\beta_Y$ holds if and only if $\epsilon_{GY} \circ L\beta_Y^{-1} = G\epsilon_Y \circ (\epsilon_{GLRY} \circ L\beta_{LRY}^{-1} \circ L\eta_{RY})$ holds which in turn is equivalent to commutativity of the outer part of the following diagram.



④ commutes by applying LF to the second unit-counit equation (2.3.3), ⑤ due to the fact that β^{-1} is a natural transformation and ⑥ because ε is a natural transformation. \square

Remark 3.1.3 We immediately make the following observations about Theorem 3.1.2.

1. Due to the fact that $\text{CoAlg}(F) \cong \text{Alg}(F^{\text{op}})$, where F^{op} is the opposite functor to F , we can apply the theorem to obtain liftings to algebras.
2. If $(L \dashv R, \eta, \varepsilon)$ is an equivalence [a dual equivalence] of categories then $(\bar{L} \dashv \bar{R}, \eta, \varepsilon)$ is an equivalence [a dual equivalence] of categories.

3.2 Nondeterministic Automata and Determinization

Within this section we will first shortly recall how deterministic (DA), nondeterministic (NA) and codeterministic (CDA) automata can be modeled as coalgebras in suitable categories. We will then consider adjunctions between these categories and apply our theorem to obtain a lifting. Via this we will recover the (co)determinization of an automaton via the powerset construction.

The content of this (and the following) section is summarized in the diagram of categories and functors in Figure 3.2.1. While DA live in Set , NA can be seen as arrows in Rel and CDA as arrows in Set^{op} (see Section 3.2.1). Furthermore in Section 3.3 we will in addition consider deterministic join automata (DJA) which live in the category of complete join semilattices (JSL), see Sections 3.3.1 and 3.3.2. Between these categories of coalgebras there are four adjunctions, which will be treated in the following sections.

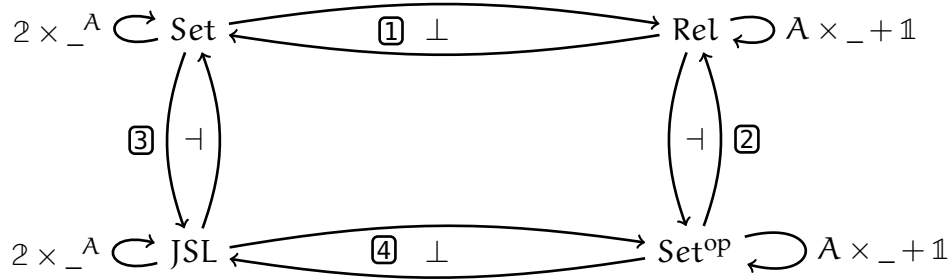


Figure 3.2.1: Four basic adjunctions and automata endofunctors

For the rest of this and the following section let A denote an alphabet, i.e., a finite set of labels. As pointed out before in a coalgebraic treatment of labeled

transition systems, one usually omits initial states and the state spaces are not required to be finite.

3.2.1 Automata as Coalgebras

As we have discussed in the Preliminaries (in Section 2.4.1), some automata have several different coalgebraic models where both the functor as well as the underlying category may be different. Thus let us now first fix the coalgebraic models we will use in this chapter.

Deterministic Automata. In the category \mathbf{Set} of sets and functions, we model deterministic automata as coalgebras for the functor $\mathcal{P} \times _^A$. We represent a deterministic automaton with state space X and alphabet A as a coalgebra $c = \langle o, s \rangle: X \rightarrow \mathcal{P} \times X^A$ where each state $x \in X$ is mapped to a tuple $(o(x), s(x))$ in which the output flag $o(x) \in \{0, 1\}$ determines whether x is final ($o(x) = 1$) or not ($o(x) = 0$) and the successor function $s(x): A \rightarrow X$ determines for each letter $a \in A$ the unique a -successor $s(x)(a) \in X$ of the state x . We thus define the category of deterministic automata and automata morphisms to be $\mathbf{DA} := \mathbf{CoAlg}(\mathcal{P} \times _^A: \mathbf{Set} \rightarrow \mathbf{Set})$.

Nondeterministic Automata. We model a nondeterministic automaton by a coalgebra for the functor¹ $A \times _ + \mathbb{1}$ in \mathbf{Rel} . Given a set X of states, and a coalgebra $c: X \leftrightarrow A \times X + \mathbb{1}$, each state $x \in X$ is in relation with \checkmark if and only if it is a final state. For any letter $a \in A$ the $y \in X$ such that $(x, (a, y)) \in c$ are the a -successor(s) (one, multiple or none) of x . We thus define the category of nondeterministic automata and automata morphisms to be $\mathbf{NA} := \mathbf{CoAlg}(A \times _ + \mathbb{1}: \mathbf{Rel} \rightarrow \mathbf{Rel})$.

Codeterministic Automata. Given a set X of states, a codeterministic (backwards deterministic) automaton (CDA) is given by a function $c: A \times X + \mathbb{1} \rightarrow X$ where $c(\checkmark) \in X$ is the unique final state and for each pair $(a, x) \in A \times X$ the unique a -predecessor of x is $c(a, x)$. Hence we can model them as coalgebras for the functor $A \times _ + \mathbb{1}$ on $\mathbf{Set}^{\mathbf{op}}$ and define the category of codeterministic automata and their morphisms to be $\mathbf{CDA} = \mathbf{CoAlg}(A \times _ + \mathbb{1}: \mathbf{Set}^{\mathbf{op}} \rightarrow \mathbf{Set}^{\mathbf{op}})$.

Note that $\mathbf{Set}^{\mathbf{op}}$ is equivalent to the category of all complete atomic boolean algebras, with boolean algebra homomorphisms. So instead of thinking of these automata as codeterministic, one could think of them as deterministic automata

¹This functor arises as an extension in the sense of Definition 2.3.42 of the \mathbf{Set} -functor $A \times _ + \mathbb{1}$ to the Kleisli category of the powerset monad.

with a rich algebraic structure on the states, even richer than the deterministic join automata introduced in Section 3.3.

Codeterministic automata have also been studied in the context of Brzozowski's minimization algorithm as *átomata* [BT11].

An example automaton is shown in Figure 3.3.1 (right).

3.2.2 Determinization of Nondeterministic Automata

Let us reconsider the Kleisli adjunction (adjunction ① of Figure 3.2.1) between **Set** and **Rel** which we presented in Example 2.3.32. We aim at applying Theorem 3.1.2 to this adjunction to get a lifting and claim that this will yield the well known powerset construction to determinize nondeterministic automata.

We will use Theorem 3.1.2 (2) to do so, because it is much easier to verify than the first condition. Recall that, by Theorem 3.1.2 (2), for a lifting to exist it is sufficient to define a natural isomorphism $\beta: \mathcal{P}(A \times _ + \mathbb{1}) \Rightarrow 2 \times (\mathcal{P}_)^A$. We define for every set X the function $\beta_X = \langle o_X, s_X \rangle: \mathcal{P}(A \times X + \mathbb{1}) \rightarrow 2 \times (\mathcal{P}X)^A$ where

$$o_X(S) = \begin{cases} 1, & \text{if } \checkmark \in S \\ 0, & \text{else} \end{cases} \quad (3.2.1)$$

$$s_X(S): A \rightarrow \mathcal{P}X, \quad s(S)(a) = \{x \in X \mid (a, x) \in S\} \quad (3.2.2)$$

for every set $S \in \mathcal{P}(A \times X + \mathbb{1})$. The inverse function $\beta_X^{-1}: 2 \times (\mathcal{P}X)^A \rightarrow \mathcal{P}(A \times X + \mathbb{1})$ is given by

$$\beta_X^{-1}(o, s) := \{\checkmark \mid o = 1\} \cup \bigcup_{a \in A} \{a\} \times s(a) \quad (3.2.3)$$

for every $(o, s) \in 2 \times (\mathcal{P}X)^A$. The proof that this is indeed a natural isomorphism is a straightforward but lengthy calculation and can be found in Appendix A.1. By Theorem 3.1.2.2 we obtain a lifting. We calculate the natural transformation $\alpha: 2 \times (_)^A \Rightarrow A \times _ + \mathbb{1}$ by using (3.1.6) to obtain for every set X the relation $\alpha_X: 2 \times X^A \leftrightarrow A \times X + \mathbb{1}$ given by

$$\alpha_X = \left\{ \left((1, s), \checkmark \right), \left((o, s), (a, s(a)) \right) \mid o \in 2, s \in X^A, a \in A \right\}. \quad (3.2.4)$$

With these preparations at hand we can now construct the lifted functors. The new left adjoint $\bar{L}: \mathbf{DA} \rightarrow \mathbf{NA}$ maps a DJA $c: X \rightarrow 2 \times X^A$ to the NA

$\bar{L}(c): X \leftrightarrow A \times X + \mathbb{1}$ which is given by²

$$\bar{L}(c) = \left\{ (x, \checkmark) \mid \begin{array}{l} x \in X \\ \pi_1 \circ c(x) = 1 \end{array} \right\} \cup \left\{ (x, (a, \pi_2 \circ c(x)(a))) \mid \begin{array}{l} x \in X \\ a \in A \end{array} \right\} \quad (3.2.5)$$

which is simply the same automaton, but interpreted as a nondeterministic one.

The lifted right adjoint $\bar{R}: \text{NA} \rightarrow \text{DA}$ maps a nondeterministic automaton $d: Y \leftrightarrow A \times Y + \mathbb{1}$ to the deterministic automaton $\bar{R}(d) = \langle o, s \rangle: \mathcal{P}Y \rightarrow 2 \times (\mathcal{P}Y)^A$. A state of this new automaton is just a set of states $Q \in \mathcal{P}Y$ of the original automaton. For each such Q the tuple $\bar{R}(d)(Q) = (o(Q), s(Q))$ is given as follows. We have

$$o(Q) = \begin{cases} 1, & \text{if there is a } q \in Q \text{ such that } (q, \checkmark) \in d \\ 0, & \text{else} \end{cases} \quad (3.2.6)$$

i.e., Q is final if and only if one of the original states in Q is final. Moreover, the unique successors of Q are given by

$$s(Q): A \rightarrow \mathcal{P}Y, \quad s(Q)(a) = \{y \in Y \mid \exists q \in Q : (q, (a, y)) \in d\}$$

which we can easily identify to be exactly the definition of the transition function of the usual powerset automaton construction. Let us demonstrate this with a concrete example.

Example 3.2.1 (Determinization of a Nondeterministic Automaton) We consider the nondeterministic automaton with state space $Y = \{y_1, y_2\}$ and input alphabet $A = \{a, b\}$ as depicted in Figure 3.2.2 on the left. In our coalgebraic

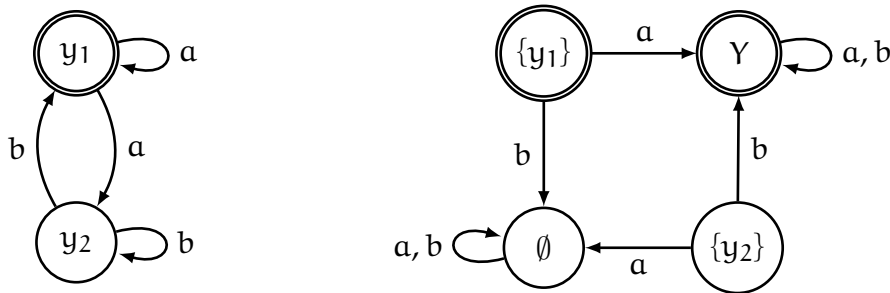


Figure 3.2.2: An NA (left) and its determinization (right)

model in Rel this automaton is given by the relation $d \subseteq Y \times (A \times Y + \mathbb{1})$ where

$$d := \{(y_1, \checkmark), (y_1, (a, y_1)), (y_1, (a, y_2)), (y_2, (b, y_2)), (y_2, (b, y_1))\}.$$

² $\pi_1: 2 \times X^A \rightarrow 2$ and $\pi_2: 2 \times X^A \rightarrow X^A$ are the projections of the product.

If we construct its determinization as presented above, we obtain the deterministic automaton depicted in Figure 3.2.2 on the right. Formally, this is the coalgebra $\langle o, s \rangle := \bar{R}(d): \mathcal{P}Y \rightarrow 2 \times (\mathcal{P}Y)^A$ where o and s are defined as follows.

state x	final state? $o(x)$	a-successor $s(x)(a)$	b-successor $s(x)(b)$
\emptyset	0	\emptyset	\emptyset
$\{y_1\}$	1	Y	\emptyset
$\{y_2\}$	0	\emptyset	Y
Y	1	Y	Y

3.2.3 Codeterminization of Nondeterministic Automata

Let us now consider adjunction $\textcircled{2}$ of Figure 3.2.1 between Rel and Set^{op} which we automatically obtain by dualizing the Kleisli adjunction between Set and Rel from Example 2.3.32 and the fact that Rel is a self-dual category.

The left adjoint $L: \text{Rel} \rightarrow \text{Set}^{\text{op}}$ maps a set X to its powerset $\mathcal{P}X$ and a relation $f: X \leftrightarrow Y$ to the function $Lf: \mathcal{P}X \leftarrow \mathcal{P}Y$ given by, for every $S \in \mathcal{P}Y$, $(Lf)(S) = \{x \in X \mid \exists y \in S : (x, y) \in f\}$. The right adjoint $R: \text{Set}^{\text{op}} \rightarrow \text{Rel}$ is the inclusion, i.e., it maps a set X to itself and a function $f: X \leftarrow Y$ to the corresponding relation $f: X \leftrightarrow Y$. The unit η consists of all the relations $\eta_X: X \leftrightarrow \mathcal{P}X$ defined via $(x, S) \in \eta_X$ if and only if $x \in S$ and the counit ε is given by all the functions $\varepsilon_X: \mathcal{P}X \leftarrow X$ mapping each $x \in X$ to the singleton set $\{x\}$.

We proceed to define a lifting as before by specifying a natural isomorphism $\beta: A \times _ + \mathbb{1} \Rightarrow A \times _ + \mathbb{1}$. The obvious choice is to let β_X be the identity relation on $A \times X + \mathbb{1}$ which indeed yields a natural isomorphism. Moreover, using (3.1.6) we obtain the natural transformation $\alpha: \mathcal{P}(A \times _ + \mathbb{1}) \Rightarrow A \times \mathcal{P}_ + \mathbb{1}$ where for each set X the function $\alpha_X: \mathcal{P}(A \times X + \mathbb{1}) \leftarrow A \times \mathcal{P}X + \mathbb{1}$ is given by $\alpha(\checkmark) = \mathbb{1}$ and $\alpha(a, S) = \{a\} \times S$ for every $(a, S) \in A \times \mathcal{P}X$.

The lifted left adjoint $\bar{L}: \text{NA} \rightarrow \text{CDA}$ performs codeterminization: Given an NA $c: X \leftrightarrow A \times X + \mathbb{1}$ we obtain a CDA $\bar{L}(c): \mathcal{P}X \leftarrow A \times \mathcal{P}X + \mathbb{1}$ where \checkmark is mapped to the set $\{x \in X \mid (x, \checkmark) \in c\}$, i.e., the unique final state of the new automaton is the set of all final states of the original automaton. Given a set of states $S \in \mathcal{P}X$ and a letter $a \in A$ the a -predecessor of S is the set

$$\bar{L}(c)(a, S) = \{x \in X \mid \exists y \in S : (x, (a, y)) \in c\} \quad (3.2.7)$$

containing all the a -predecessors of the states in S . We conclude that the new automaton is indeed a codeterministic automaton which is (language) equivalent to the original one.

While in the previous example the lifted left adjoint was trivial (as was the original left adjoint), in this case we obtain a trivial lifted right adjoint

$\bar{R}: \text{CDA} \rightarrow \text{NA}$: it “interprets” a CDA $d: Y \leftarrow A \times Y + \mathbb{1}$ as NA, i.e., as the corresponding relation $\bar{R}(d): Y \leftrightarrow A \times Y + \mathbb{1}$.

As before, we illustrate the non-trivial construction (this time the application of the lifted left adjoint) on a concrete example.

Example 3.2.2 (Codeterminization of a Nondeterministic Automaton) We consider the nondeterministic automaton with state space $X = \{x_1, x_2\}$ and input alphabet $A = \{a, b\}$ as depicted in Figure 3.2.3 on the left. In our coalge-

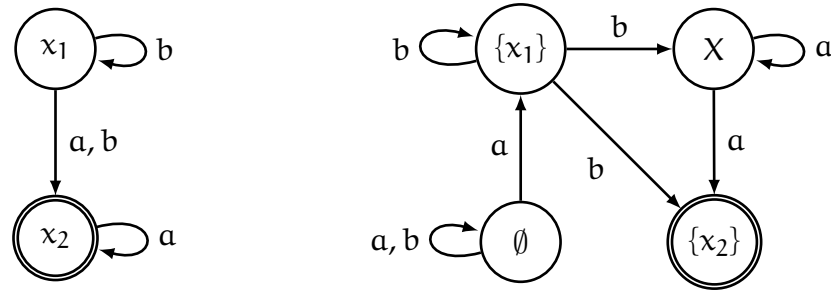


Figure 3.2.3: An NA (left) and its codeterminization (right)

braic model in Rel this automaton is given by the relation $c \subseteq X \times (A \times X + \mathbb{1})$ where

$$c := \{(x_2, \checkmark), (x_1, (a, x_2)), (x_1, (b, x_1)), (x_1, (b, x_2)), (x_2, (a, x_1))\}.$$

If we construct its determinization as presented above, we obtain the codeterministic automaton depicted in Figure 3.2.3 on the right. Formally, this is the coalgebra $d := \bar{L}(c): \mathcal{P}X \leftarrow A \times \mathcal{P}X + \mathbb{1}$ defined as in the following tabular.

state y	final, i.e., $c(\checkmark) = y$	a -predecessor $d(a, y)$	b -predecessor $d(b, y)$
\emptyset	no	\emptyset	\emptyset
$\{x_1\}$	no	\emptyset	$\{x_1\}$
$\{x_2\}$	yes	X	$\{x_1\}$
X	no	X	$\{x_1\}$

While predecessors are by construction unique in this codeterminization, it is clearly not a usual (forward) deterministic automaton.

3.3 Deterministic Join Automata

We will now try to take a different perspective to look at powerset automata instead of just considering them to be determinized nondeterministic automata. In order to do that we briefly recall the notion of complete join semilattices and the corresponding category.

3.3.1 Complete Join Semilattices

A complete join semilattice is a partially ordered set X such that for every (possibly infinite) set $S \in \mathcal{P}X$ there is a least upper bound, called *join* and denoted by $\sqcup S$. If Y is another join semilattice we call a function $f: X \rightarrow Y$ *join-preserving* if, for all S , it satisfies $f(\sqcup S) = \sqcup \{f(s) \mid s \in S\}$. The join semilattices and the join-preserving functions form a category which we will denote by \mathbf{JSL} . It is easy to see that this category is isomorphic to the Eilenberg-Moore category for the powerset monad on \mathbf{Set} .

If we equip the set $2 = \{0, 1\}$ with the partial order $0 \leq 1$, we get a complete join semilattice with $\sqcup \emptyset = 0$, $\sqcup \{0\} = 0$, $\sqcup \{1\} = 1$ and $\sqcup 2 = 1$.

The product of two join semilattices X and Y is the cartesian product of the base sets equipped with a partial order given by $(x_1, y_1) \leq (x_2, y_2)$ if and only if $x_1 \leq x_2$ and $y_1 \leq y_2$ for all $x_1, x_2 \in X$, $y_1, y_2 \in Y$ and analogously, given a set X we can equip X^A with a partial order based on a given one on X by defining for $f, g \in X^A$ that $f \leq g$ if and only if $f(a) \leq g(a)$ for every $a \in A$. This is a complete join semilattice if X is. Given a subset $F \subseteq X^A$ its join is given by $\sqcup F: A \rightarrow X$, $\sqcup F(a) = \sqcup \{f(a) \mid f \in F\}$.

3.3.2 Deterministic Join Automata

We can interpret a coalgebra $c: X \rightarrow 2 \times X^A$ for the functor $2 \times _^A$ on \mathbf{JSL} as a deterministic automaton just as we did before on \mathbf{Set} . Since the arrows of \mathbf{JSL} are join-preserving functions, such an automaton possesses a certain additional property. Given a set $S \in \mathcal{P}X$ of states, we know that there is a *join-state* $\sqcup S$. By the join-preserving property of the transition function c we know that $c(\sqcup S) = \sqcup \{c(x) \mid x \in S\}$ and we conclude that $\sqcup S$ is final if and only if one of the states $x \in S$ is final and moreover any transition of an $x \in S$ can be “simulated” (see below) by $\sqcup S$. We define the category $\mathbf{DJA} := \mathbf{CoAlg}(2 \times _^A: \mathbf{JSL} \rightarrow \mathbf{JSL})$ and call its objects *deterministic join automata*.

Example 3.3.1 (A Simple Deterministic Join Automaton) Take a look at Figure 3.3.1. If we equip the set $X = \{\perp, u, x, y, \top\}$ with the partial order given by the Hasse diagram on the left we obtain a complete join semilattice. The diagram in the middle shows a deterministic join automaton on this join semilattice. Note that the join of two final states is again final and that for every pair of states and alphabet symbol a , the a -successor of the join of the states is the join of the a -successors. This implies a general property of \mathbf{DJA} that for every subset of states there exists a state accepting the union of the languages of the given states.

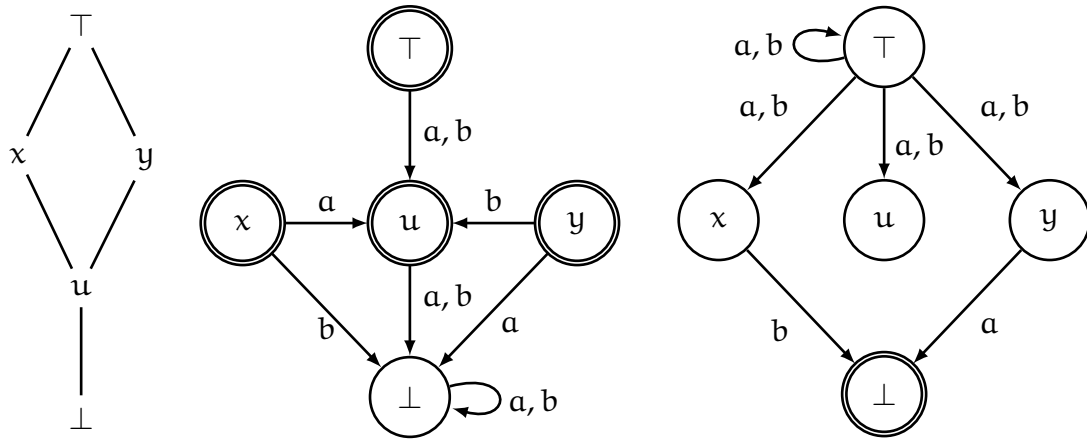


Figure 3.3.1: Hasse diagram of a complete join semilattice, a deterministic join automaton and its codeterminization (from left to right)

3.3.3 Determinization of Deterministic Automata

We will now consider adjunction ③ of Figure 3.2.1 in order to transform DJA into DAs and vice versa. Given a conventional DA, a suitable algorithm to obtain a DJA is (again) the powerset determinization construction – this time employed to an already deterministic automaton. We will see that this is a reasonable construction in the sense that it arises from an adjunction between **Set** and **JSL**. As said before, the category of complete join semilattices is isomorphic to the Eilenberg-Moore category for the powerset monad on **Set**. The theory of adjunctions gives us a generic construction of an adjunction (see Definition 2.3.41) which we will now spell out again using the aforementioned isomorphism between $\mathcal{EM}(\mathcal{P})$ and **JSL**.

The left adjoint $L: \mathbf{Set} \rightarrow \mathbf{JSL}$ maps any set X to $\mathcal{P}X$ which is partially ordered by set inclusion. The join operation is set theoretic union and it is easy to see that we indeed obtain a complete join semilattice. Any function $f: X \rightarrow Y$ is mapped to its image map $f[\cdot]: \mathcal{P}X \rightarrow \mathcal{P}Y$ which we can easily identify as join- (i.e., union-)preserving function. The right adjoint $R: \mathbf{JSL} \rightarrow \mathbf{Set}$ takes a complete join semilattice to its base set and forgets about the order and the join operation. Analogously, a join-preserving function is just considered as a function. The unit of the adjunction is given, for every set X , by the function $\eta_X: X \rightarrow \mathcal{P}X, \eta_X(x) = \{x\}$. The counit consists of the join-preserving functions $\varepsilon_{(Y, \sqcup)}: (\mathcal{P}Y, \cup) \rightarrow (Y, \sqcup)$ mapping each set $S \in \mathcal{P}Y$ to its join $\sqcup S$ in Y .

In order to obtain the lifting we define $\beta_{(X, \sqcup)}: 2 \times X^A \rightarrow 2 \times X^A$ to be the identity function on $2 \times X^A$ for every join semilattice (X, \sqcup) which obviously yields a

natural isomorphism β . Using (3.1.6) we construct the natural transformation α where for each set X the join preserving function $\alpha_X: \mathcal{P}(2 \times X^A) \rightarrow 2 \times (\mathcal{P}X)^A$ is given by, for every $S \in \mathcal{P}(2 \times X^A)$,

$$\alpha_X(S) = \left(\bigsqcup \{o \mid (o, s) \in S\}, \bigsqcup \{s \mid (o, s) \in S\} \right). \quad (3.3.1)$$

The lifted left adjoint $\bar{L}: \text{DA} \rightarrow \text{DJA}$ performs the powerset construction on a deterministic automaton: For a deterministic automaton $c: X \rightarrow 2 \times X^A$ the deterministic join automaton $\bar{L}(c): \mathcal{P}X \rightarrow 2 \times (\mathcal{P}X)^A$ is given by, for all $S \in \mathcal{P}X$,

$$\bar{L}(c)(S) = \left(\bigsqcup \{\pi_1(c(x)) \mid x \in S\}, \bigsqcup \{\pi_2(c(x)) \mid x \in S\} \right). \quad (3.3.2)$$

The lifted right adjoint $\bar{R}: \text{DJA} \rightarrow \text{DA}$ takes a DJA and interprets it as DA by forgetting about its join property.

Again we illustrate our construction on a simple example.

Example 3.3.2 (Transforming a DA into a DJA) We consider the deterministic automaton with state space $X = \{x_1, x_2\}$ and input alphabet $A = \{a, b\}$ as depicted in Figure 3.3.2 on the left. In our coalgebraic model in Set this

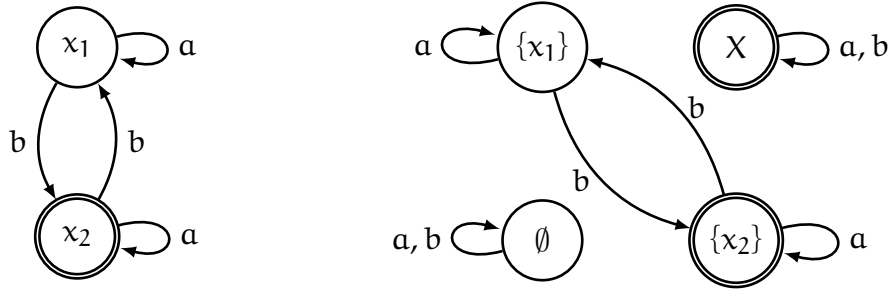


Figure 3.3.2: A DA (left) and its transformation to a DJA (right)

automaton is given by the function $c = \langle o_c, s_c \rangle: X \rightarrow 2 \times X^A$ with values as presented in the tabular below.

state x	final state? $o_c(x)$	a-successor $s_c(x)(a)$	b-successor $s_c(x)(b)$
x_1	0	x_1	x_2
x_2	1	x_2	x_1

If we transform it into a DJA as presented above, we obtain the automaton depicted in Figure 3.3.2 on the right. Formally, this is the function $d = \langle o_d, s_d \rangle := \bar{L}(c): \mathcal{P}X \rightarrow 2 \times (\mathcal{P}X)^A$ defined as in the following tabular.

state y	final state? $o_d(y)$	a-successor $s_d(y)(a)$	b-successor $s_d(y)(b)$
\emptyset	0	\emptyset	\emptyset
$\{x_1\}$	0	$\{x_1\}$	$\{x_2\}$
$\{x_2\}$	1	$\{x_2\}$	$\{x_1\}$
X	1	X	X

Apparently, the construction contains the original automaton and just adds the join-states. However, these are not reachable from the singleton states.

3.3.4 Codeterminization of Deterministic Join Automata

Finally, we will describe a construction translating DJA into CDA, based on adjunction ④ of Figure 3.2.1. The unit of the adjunction (which must be join-preserving) maps every element to the complement (!) of its upward-closure (more details are given below).

The left adjoint $L: \text{JSL} \rightarrow \text{Set}^{\text{op}}$ maps any join semilattice (X, \sqcup) to its base set X and each join-preserving function $f: (X, \sqcup) \rightarrow (Y, \sqcup)$ to the Set^{op} -arrow

$$Lf: X \leftarrow Y, \quad Lf(y) = \bigsqcup \{x \in X \mid f(x) \sqsubseteq y\}. \quad (3.3.3)$$

The right adjoint $R: \text{Set}^{\text{op}} \rightarrow \text{JSL}$ maps a set X to its powerset $\mathcal{P}X$ equipped with the subset order, i.e., to the join semilattice $(\mathcal{P}X, \cup)$ and each Set^{op} -arrow $f: X \leftarrow Y$ to the reverse image $f^{-1}[\cdot]: \mathcal{P}X \rightarrow \mathcal{P}Y$. The unit of this adjunction is given by the join-preserving functions

$$\eta_{(X, \sqcup)}: (X, \sqcup) \rightarrow (\mathcal{P}(X), \cup), \quad x \mapsto \overline{\uparrow x} = \{x' \in X \mid x' \not\sqsubseteq x\} \quad (3.3.4)$$

for every join semilattice (X, \sqcup) and the counit is given by, for every set X ,

$$\varepsilon_X: \mathcal{P}X \leftarrow X, \quad x \mapsto \overline{\{x\}}. \quad (3.3.5)$$

We construct a natural isomorphism $\beta: (\mathcal{P}(A \times _ + \mathbb{1}), \cup) \Rightarrow (2 \times (\mathcal{P}_)^A, \sqcup)$ in order to get a lifting. For every join semilattice (X, \sqcup) we take β_X to be the same function as defined by Equations (3.2.1) and (3.2.2) of our first example given in Section 3.2.2 and claim that this is a join-preserving function: for two sets $Q_1, Q_2 \in \mathcal{P}(A \times X + \mathbb{1})$ let $(o, s) := \beta_X(Q_1 \cup Q_2)$ and $(o_i, s_i) = \beta_X(Q_i)$ for $i \in \{1, 2\}$ then we have $o = \chi_{Q_1 \cup Q_2}(\checkmark) = \max\{\chi_{Q_1}(\checkmark), \chi_{Q_2}(\checkmark)\} = \max\{o_1, o_2\} = o_1 \sqcup o_2$ and for each $a \in A$ we have

$$\begin{aligned} s(a) &= \{x \in X \mid (a, x) \in Q_1 \cup Q_2\} \\ &= \{x \in X \mid (a, x) \in Q_1\} \cup \{x \in X \mid (a, x) \in Q_2\} = s_1(a) \cup s_2(a) \end{aligned}$$

which can be generalized to arbitrary unions.

We calculate $\alpha: 2 \times _{}^A \Leftarrow A \times _{} + \mathbb{1}$ where for every join semilattice (X, \sqcup) the function $\alpha_{(X, \sqcup)}$ is given by $\alpha_{(X, \sqcup)}(\checkmark) = (0, (s_{\checkmark}: A \rightarrow X, s_{\checkmark}(a) = \top))$ and

$$\alpha_{(X, \sqcup)}((a, x)) = \left(1, \left(s_{(a, x)}: A \rightarrow X, s_{(a, x)}(a') = \begin{cases} x, & a' = a \\ \top, & a' \neq a \end{cases} \right) \right). \quad (3.3.6)$$

The lifted left adjoint $\bar{L}: \text{DJA} \rightarrow \text{CDA}$ maps a DJA $c: (X, \sqcup) \rightarrow (2 \times X^A, \sqcup)$ to the CDA $\bar{L}c: X \leftarrow A \times X + \mathbb{1}$ whose unique final state is the join of the non-final states of the original automaton, i.e., $\bar{L}c(\checkmark) = \sqcup \{x' \in X \mid \pi_1(c(x')) = 0\}$. For every action $a \in A$ and every state $x \in X$ the unique a -predecessor of x is the join of all the states of the original automaton whose a -successor is less or equal to x , i.e., $\bar{L}c((a, x)) = \sqcup \{x' \in X \mid \pi_2(c(x'))(a) \sqsubseteq x\}$.

The lifted right adjoint $\bar{R}: \text{CDA} \rightarrow \text{DJA}$ maps a CDA $d: Y \leftarrow A \times Y + \mathbb{1}$ (which can also be regarded as nondeterministic automaton) to its determinization $\bar{R}(d): (\mathcal{P}Y, \cup) \rightarrow (2 \times (\mathcal{P}Y)^A, \sqcup)$ via the usual powerset construction, i.e., for every $S \in \mathcal{P}Y$ we have $\bar{R}(d)(S) = \beta_Y \circ d^{-1}[S]$. Since the reverse image of any function preserves arbitrary unions, this is indeed a DJA.

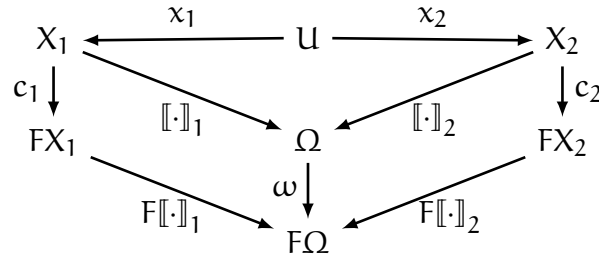
Example 3.3.3 (Codeterminization of a DJA) We take another look at Figure 3.3.1. The DJA of Example 3.3.1 (in the middle) is transformed into a CDA with the same state set $X = \{\perp, x, y, u, \top\}$ (the diagram on the right). Its unique final state is \perp (the join of the non-final states) and the unique a -predecessor of a state is the join of the previous a -predecessors, for instance the new a -predecessor of \perp is y (the join of \perp, u, y). If we transfer this automaton into a DJA with state set $\mathcal{P}X$ via the right adjoint the unit $\eta_{(X, \sqcup)}$ maps every state to the complement of its upward-closure. For instance state x is mapped to $\{\perp, u, y\}$.

3.4 Checking Behavioral Equivalences

In this final part we will now show how the results on adjunctions can be used to check behavioral equivalences. Since our coalgebras do not necessarily live in Set , where we could address elements of a carrier set (like we did in Definition 2.4.11), we use the following alternative definition, where we specify whether two *arrows* are behaviorally equivalent. This is reminiscent of equipping a coalgebra with start states, similar to the initial states of an automaton.

Definition 3.4.1 (Behavioral Equivalence) Let \mathcal{C} be a category, $F: \mathcal{C} \rightarrow \mathcal{C}$ be an endofunctor such that a final F -coalgebra $\omega: \Omega \rightarrow F\Omega$ exists. Furthermore let $c_1: X_1 \rightarrow FX_1$ and $c_2: X_2 \rightarrow FX_2$ be two F -coalgebras and U be a \mathcal{C} -object. We

say that two \mathcal{C} -arrows $x_1: U \rightarrow X_1$, $x_2: U \rightarrow X_2$ are *behaviorally equivalent* (in symbols $x_1 \sim_F^{c_1, c_2} x_2$), whenever the diagram below commutes.



In this diagram the arrows $[\cdot]_1: c_1 \rightarrow \omega$ and $[\cdot]_2: c_2 \rightarrow \omega$ are the unique coalgebra homomorphisms into the final coalgebra.

In \mathbf{Set} the choice for U will typically be a singleton set and then the problem reduces to asking whether two given states are behaviorally equivalent.

Assume that we have an adjunction $(L \dashv R, \eta, \epsilon): \mathcal{C} \rightarrow \mathcal{D}$ that is lifted to coalgebras as specified in Definition 3.1.1. Since \bar{R} is a right adjoint, it preserves limits [Awo06, Proposition 9.14], specifically it preserves the final coalgebra. Let us now take another look at the diagram in Figure 3.2.1 (page 71): It can easily be determined that A^* , the set of all finite words, is the carrier of the final coalgebra of $A \times _ + \mathbb{1}$ in \mathbf{Set}^{op} . Via the right adjoint, this translates to the carrier set A^* in \mathbf{Rel} , where the arrow $[\cdot]$ into the final coalgebra is a relation, relating each state with the words that are accepted by it (this final coalgebra, which captures trace semantics for nondeterministic automata, is used in the Kleisli approach to trace semantics [HJS07]). The final coalgebra can also be transferred into \mathbf{JSL} and \mathbf{Set} , where it has the carrier set $\mathcal{P}(A^*)$ of all languages over A .

Hence, the adjunctions allow to construct final coalgebras and to transfer results about final semantics from other categories. Furthermore, it is possible to check behavioral equivalence in a different category, by translating queries via the adjunction.

Theorem 3.4.2 Let \mathcal{C}, \mathcal{D} be categories, $F: \mathcal{C} \rightarrow \mathcal{C}$ and $G: \mathcal{D} \rightarrow \mathcal{D}$ be endofunctors, $(L \dashv R, \eta, \epsilon): \mathcal{C} \rightarrow \mathcal{D}$ be an adjunction together with a lifting in the sense of Definition 3.1.1, i.e., an adjunction $(\bar{L} \dashv \bar{R}, \eta, \epsilon): \mathbf{CoAlg}(F) \rightarrow \mathbf{CoAlg}(G)$. Furthermore assume that a final G -coalgebra exists and that R is faithful.

Let $d_1: Y_1 \rightarrow GY_1$, $d_2: Y_2 \rightarrow GY_2$ be two G -coalgebras and let $y_1: U \rightarrow Y_1$, $y_2: U \rightarrow Y_2$ be two arrows in \mathcal{D} . Then the following equivalence holds.

$$y_1 \sim_G^{d_1, d_2} y_2 \iff Ry_1 \sim_F^{\bar{R}d_1, \bar{R}d_2} Ry_2$$

Proof. We show both implications separately.

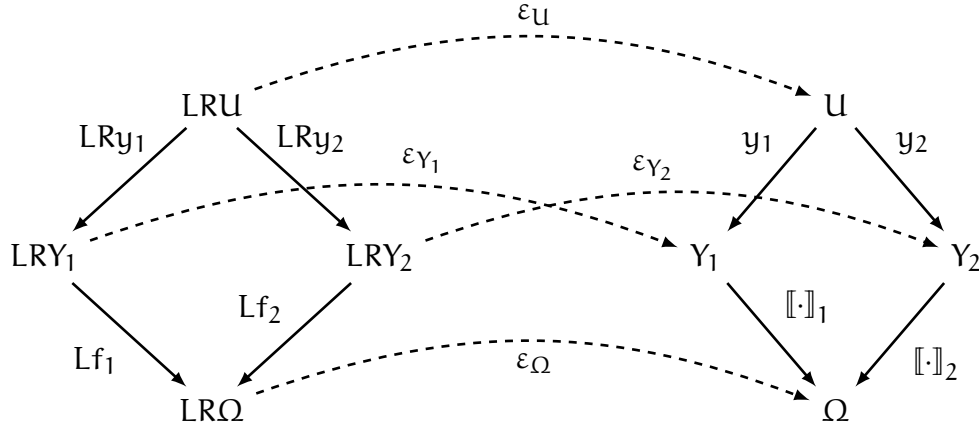
\Rightarrow Whenever $y_1 \sim_F^{d_1, d_2} y_2$ we have that $\llbracket \cdot \rrbracket_1 \circ y_1 = \llbracket \cdot \rrbracket_2 \circ y_2$. Applying R to the diagram yields $R\llbracket \cdot \rrbracket_1 \circ Ry_1 = R\llbracket \cdot \rrbracket_2 \circ Ry_2$. Moreover, $R\llbracket \cdot \rrbracket_1$ and $R\llbracket \cdot \rrbracket_2$ are coalgebra homomorphisms from $\bar{R}d_1, \bar{R}d_2$ to $\bar{R}\omega$, which is the final F -coalgebra, and thus are unique with this property. Hence $Ry_1 \sim_F^{\bar{R}d_1, \bar{R}d_2} Ry_2$.

\Leftarrow Assume $Ry_1 \sim_F^{\bar{R}d_1, \bar{R}d_2} Ry_2$. Then we have $f_1 \circ Ry_1 = f_2 \circ Ry_2$ where f_1, f_2 are the unique coalgebra homomorphisms from $\bar{R}d_1, \bar{R}d_2$ to $\bar{R}\omega$. We apply the left adjoint L and get $Lf_1 \circ LRy_1 = Lf_2 \circ LRy_2$.

We have to show that $\llbracket \cdot \rrbracket_1 \circ y_1 = \llbracket \cdot \rrbracket_2 \circ y_2$ and we prove commutativity by prefixing with the counit $\varepsilon_U: LRU \rightarrow U$. First, note that $\llbracket \cdot \rrbracket_1 \circ \varepsilon_{Y_1}$ is a coalgebra homomorphism from $\bar{L}Rd_1$ into the final coalgebra and so is $\varepsilon_\Omega \circ Lf_1$. Since such a morphism is unique we have $\llbracket \cdot \rrbracket_1 \circ \varepsilon_{Y_1} = \varepsilon_\Omega \circ Lf_1$. Similarly $\llbracket \cdot \rrbracket_2 \circ \varepsilon_{Y_2} = \varepsilon_\Omega \circ Lf_2$. Hence

$$\begin{aligned} \llbracket \cdot \rrbracket_1 \circ y_1 \circ \varepsilon_U &= \llbracket \cdot \rrbracket_1 \circ \varepsilon_{Y_1} \circ LRy_1 = \varepsilon_\Omega \circ Lf_1 \circ LRy_1 = \varepsilon_\Omega \circ L(f_1 \circ Ry_1) \\ &= \varepsilon_\Omega \circ L(f_2 \circ Ry_2) = \varepsilon_\Omega \circ Lf_2 \circ LRy_2 = \llbracket \cdot \rrbracket_2 \circ \varepsilon_{Y_2} \circ LRy_2 = \llbracket \cdot \rrbracket_2 \circ y_2 \circ \varepsilon_U \end{aligned}$$

The situation is depicted below.



Due to the right equation in (2.3.3) of Definition 2.3.31 we know that $R\varepsilon_U$ is a split epi and hence an epi. Epis are reflected by faithful functors and so ε_U is an epi. We can conclude that $\llbracket \cdot \rrbracket_1 \circ y_1 = \llbracket \cdot \rrbracket_2 \circ y_2$, as required. \square

In all our examples the right adjoint R is faithful. If this is the case and the final coalgebra exists, this allows us to check behavioral equivalence in a different category, where this might be easier or more straightforward. The classical example is of course the lifted adjunction between Set and Rel . In order to check language equivalence for nondeterministic automata, the standard

technique is to determinize them via the right adjoint into Set . Then, language equivalence can be checked on the powerset automaton, where it is bisimilarity.

3.5 Conclusion

We have identified and analyzed sufficient conditions which allow to lift an adjunctions between two categories to an adjunctions between categories of coalgebras. Moreover, we illustrated our theory by considering several examples for such adjunction liftings where we rediscovered known algorithms and constructions. Finally, we discussed how the fact that these constructions are lifted adjoints can be used to transfer behavioral equivalence checks from one category to another.

3.5.1 Open Questions and Future Work

Several open questions remain, concerning both the examples as well as the general theory. First of all, our examples are of course strongly connected to the two canonical adjunctions giving rise to the powerset monad: One adjunction is just the Kleisli adjunction (Definition 2.3.38) and the other is the Eilenberg-Moore adjunction (Definition 2.3.41) for this monad. In this specific case (due to the fact that $\mathcal{EM}(\mathcal{P}) = \text{Rel}$ is self-dual) we easily obtain two more adjunctions by considering Set^{op} , however this will not work for any monad. Still, it would be interesting to investigate other monads and see which automata constructions are hidden underneath the corresponding Kleisli/Eilenberg-Moore adjunction.

In presence of monads and the aforementioned adjunctions, it might also be interesting to consider the comparison functor from the Kleisli to the Eilenberg-Moore category, which however is not necessarily part of an adjunction. Nevertheless, it would be interesting to find out which behavioral information can be transported over the comparison functor.

The adjunction between Rel and Set^{op} has been used in order to characterize a factorization structure that is employed for a minimization algorithm [ABH+12]. Hence, an obvious question is whether other adjunctions can be used for such algorithmic purposes, for instance for minimizing a coalgebra in one category, but using the structure of another category. It also seems plausible that up-to techniques can be explained in this way, for instance by checking language equivalence for nondeterministic automata in Rel , using the algebraic structure of JSL via the comparison functor (similar to [BP13]).

Since we have seen in Theorem 3.4.2 how to transfer equivalence checking queries through a faithful right adjoint an obvious question is if there is something similar when considering the left adjoint.

Finally, the conditions in Theorem 3.1.2 (Lifting an Adjunction to Coalgebras) are just sufficient conditions for the lifting to exist. However, it is unclear whether they are necessary or whether one can define such necessary conditions.

3.5.2 Related Work

As mentioned above, the adjunction between Rel and Set^{op} , transforming nondeterministic automata into codeterministic automata has already been considered to obtain canonical determinization/minimization constructions [ABH+12] and also to obtain coalgebraic trace semantics [HJS07].

Another line of research which uses the adjunction between Set and JSL or more general the Eilenberg-Moore adjunction (Definition 2.3.41) is the *generalized powerset construction* [SBBR13; JSS15] which gives a canonical determinization procedure for coalgebras (we have seen this construction in Section 2.4.3). We will elaborate on this a bit more in the Conclusion. Here we just note that in their work a *nondeterministic automaton* specified by a function $X \rightarrow 2 \times (\mathcal{P}X)^A$ in Set . It is then translated into a join-preserving function $\mathcal{P}X \rightarrow 2 \times (\mathcal{P}X)^A$ using a lifting of the free functor (the left adjoint of the Eilenberg Moore adjunction). However in this setting one does not obtain a lifting of the whole adjunction.

3.5.3 Final Remarks

Summing up, many ideas of this chapter are not completely new, but have already been used in various forms. However, presenting the theory strictly from the point of *adjunction lifting* and to clearly spell out what it means to preserve and reflect *behavioral equivalences* by adjoints might permit a fresh view on these ideas. In particular, the application of our theory to examples has lead us to studying the lifting of the adjunction between join semilattices and Set^{op} , which gives rise to the quite surprising and unusual construction transforming a DJA into a CDA.

Trace Semantics for Continuous Probabilistic Transition Systems

IN the global Introduction (Chapter 1) and the Preliminaries (Chapter 2) we have already discussed the Kleisli approach to trace semantics (Section 2.4.3) as proposed by Ichiro Hasuo, Bart Jacobs and Ana Sokolova [HJS06; HJS07]. We have seen that based on this approach one can obtain trace semantics for generative probabilistic transition systems with termination. These systems are exactly the coalgebras for the Set-functor $\mathcal{D}(A \times _ + \mathbb{1})$ where \mathcal{D} is the endofunctor of the of the subdistribution monad on Set. Using a Kleisli law, the aforementioned approach views a coalgebra $c: X \rightarrow \mathcal{D}(A \times X + \mathbb{1})$ as a coalgebra for an extension of the Set-endofunctor $A \times _ + \mathbb{1}$ in the Kleisli category of the subdistribution monad.

Since the subdistribution monad satisfies some non-trivial requirements, the final coalgebra of the extended functor has as carrier the set A^* of all finite words over A since this is the carrier of the initial algebra of the Set-endofunctor $A \times _ + \mathbb{1}$. The unique map into the final coalgebra assigns to each state a probability subdistribution on the set A^* of finite words, which coincides with the usual finite trace semantics of generative probabilistic systems [Sok05; vGSST95].

The original Kleisli approach [HJS06; HJS07] is restricted to *discrete* probabilistic systems, where the probability distributions always have at most countable support [Sok11]. This might seem sufficient for practical applications at first glance, but it has two important drawbacks:

- ▷ First, it apparently excludes any system that involves *uncountable state spaces* (like the examples in Section 4.3 or examples in the literature [Pan09]).
- ▷ Second, it excludes the treatment of *infinite traces*, since the set of all infinite traces is uncountable and hence needs measure theory to be treated appropriately. This is also an intuitive reason for the choice of the subdistribution monad – instead of the distribution monad – in the original approach [HJS07]: for a given state, it might always be the case that a non-zero probability mass

is associated to the infinite traces leaving this state, which – in the discrete case – cannot be specified by a probability distribution over all words.

In this chapter, we generalize the above results to *continuous* generative probabilistic systems with uncountable state spaces. In order to do so, we replace the category *Set* by the category *Meas* of measurable spaces and measurable functions and analyze traces via the final coalgebra of an extension of the *Meas*-endofunctor $A \times _ + \mathbb{1}$ to the Kleisli category of the subprobability monad.

Unlike in the original approach [HJS07] we do not derive the final coalgebra via a generic construction (building the initial algebra of the functor), but we construct it directly. Its carrier is the measurable space obtained by endowing A^* with the discrete sigma-algebra.

In a similar vein we also consider the Kleisli category of the probability monad (Giry monad) and treat the case with (using the above endofunctor and its extension) and without termination (using an extension of the *Meas*-functor $A \times _$). In the former case we obtain a coalgebra over a measurable space with base set A^∞ (finite and infinite traces over A) and in the latter with the set A^ω (infinite traces), both endowed with a non-trivial sigma algebra of cones. For completeness we also consider the case of the subprobability monad without termination, which results in the trivial final coalgebra over the empty set. In all cases we obtain the natural trace measures as instances of the generic coalgebraic theory.

Since there is no generic construction for such coalgebras, we construct the respective final coalgebras directly and show their correctness by proving that each coalgebra admits a unique homomorphism into the final coalgebra which gives rise to the trace measure. For both the existence and the uniqueness of this homomorphism we rely on the measure-theoretic extension theorem for sigma-finite pre-measures and the identity theorem.

At the end of this chapter we will further compare our approach to the original one [HJS07] and discuss why we took an alternative route.

4.1 Measure Theoretic Basics

Within this section we give a very brief introduction to measure theory and integration which just encompasses the results we will need later. For a more thorough treatment the interested reader is invited to read one of the many standard textbooks on this topic [Ash72; Els11].

Measure theory generalizes the idea of length, area or volume. Its most basic definition is that of a σ -algebra (*sigma-algebra*). Given an arbitrary set X we call

a set Σ of subsets of X a σ -algebra if and only if it contains the empty set and is closed under complement and countable union. The tuple (X, Σ) is called a *measurable space*. We will sometimes call the set X itself a measurable space, keeping in mind that there is an associated σ -algebra which we will then denote by Σ_X . Two simple examples of a σ -algebra for any set X are the *trivial σ -algebra* $\{\emptyset, X\}$ and the *discrete σ -algebra* $\mathcal{P}X$.

For any subset $\mathcal{G} \subseteq \mathcal{P}(X)$ we can always uniquely construct the smallest σ -algebra on X containing \mathcal{G} which is denoted by $\sigma_X(\mathcal{G})$. We call \mathcal{G} the *generator* of $\sigma_X(\mathcal{G})$, which in turn is called *the σ -algebra generated by \mathcal{G}* . It is known (and easy to show), that σ_X is a monotone and idempotent operator. The elements of a σ -algebra on X are called the *measurable sets* of X . Among all possible generators for σ -algebras, there are special ones, so-called *semirings of sets*.

Definition 4.1.1 (Semiring of Sets) Let X be an arbitrary set. A subset $\mathcal{S} \subseteq \mathcal{P}(X)$ is called a *semiring of sets* if it satisfies the following three properties.

1. \mathcal{S} contains the empty set, i.e., $\emptyset \in \mathcal{S}$.
2. \mathcal{S} is closed under pairwise intersection, i.e., for $A, B \in \mathcal{S}$ we always require $(A \cap B) \in \mathcal{S}$.
3. The set difference of any two sets in \mathcal{S} is the disjoint union of finitely many sets in \mathcal{S} , i.e., for any $A, B \in \mathcal{S}$ there is an $N \in \mathbb{N}$ and pairwise disjoint sets $C_1, \dots, C_N \in \mathcal{S}$ such that $A \setminus B = \bigcup_{n=1}^N C_n$.

A trivial example of such a semiring of sets (for any set X) is the set $\{\emptyset\}$ and we will encounter more interesting examples later in this chapter. Moreover, it is easy to see that every σ -algebra is a semiring of sets but the reverse is false. Please note that a semiring of sets is different from a semiring in algebra. In this chapter we will use the term *semiring* solely as short form of the term *semiring of sets*. For our purposes we will consider special semirings containing a countable cover of the base set.

Definition 4.1.2 (Countable Cover, Covering Semiring) Let \mathcal{S} be a semiring of sets. A countable sequence $(S_n)_{n \in \mathbb{N}}$ of sets in \mathcal{S} such that $\bigcup_{n \in \mathbb{N}} S_n = X$ is called a *countable cover of X (in \mathcal{S})*. If such a countable cover exists we call \mathcal{S} a *covering semiring (of sets)*.

With these basic structures at hand, we can now define pre-measures and measures. A non-negative function $\mu: \mathcal{S} \rightarrow \overline{\mathbb{R}}_+$ defined on a semiring \mathcal{S} is called a *pre-measure* on X if it assigns 0 to the empty set and is σ -additive, i.e., for a sequence $(S_n)_{n \in \mathbb{N}}$ of pairwise disjoint sets in \mathcal{S} where $(\bigcup_{n \in \mathbb{N}} S_n) \in \mathcal{S}$ we must

have

$$\mu \left(\bigcup_{n \in \mathbb{N}} S_n \right) = \sum_{n \in \mathbb{N}} \mu(S_n). \quad (4.1.1)$$

A pre-measure μ is called σ -finite if there is a countable cover $(S_n)_{n \in \mathbb{N}}$ of X in \mathcal{S} such that $\mu(S_n) < \infty$ for all $n \in \mathbb{N}$. Whenever \mathcal{S} is a σ -algebra we call μ a *measure* and the tuple (X, \mathcal{S}, μ) a *measure space*. In that case μ is said to be *finite* if and only if $\mu(X) < \infty$ and for the special cases $\mu(X) = 1$ (or $\mu(X) \leq 1$) μ is called a *probability measure* (or *subprobability measure* respectively). Measures are *monotone*, i.e., if A, B are measurable $A \subseteq B$ implies $\mu(A) \leq \mu(B)$ and *continuous*, i.e., for measurable $A_1 \subseteq A_2 \subseteq \dots \subseteq A_n \subseteq \dots$ we always have $\mu(\bigcup_{n=1}^{\infty} A_n) = \lim_{n \rightarrow \infty} \mu(A_n)$ and for measurable $B_1 \supseteq B_2 \supseteq \dots \supseteq B_n \supseteq \dots$ with $\mu(B_1) < \infty$ we have $\mu(\bigcap_{n=1}^{\infty} B_n) = \lim_{n \rightarrow \infty} \mu(B_n)$ [Ash72, 1.2.5 and 1.2.7].

Given a measurable space (X, Σ_X) , a simple and well-known probability measure, is the so-called *Dirac measure*, which we will use later. It is defined as $\delta_x^X: \Sigma_X \rightarrow [0, 1]$, and is 1 on $S \in \Sigma_X$ if and only if $x \in S$ and 0 otherwise.

The most significant theorems from measure theory which we will use in this chapter are the identity theorem and the extension theorem for σ -finite pre-measures, for which a proof can be found in standard textbooks [Els11, II.5.6 and II.5.7].

Theorem 4.1.3 (Identity Theorem) Let X be a set, $\mathcal{G} \subseteq \mathcal{P}(X)$ be a set which is closed under pairwise intersection and $\mu, \nu: \sigma_X(\mathcal{G}) \rightarrow \overline{\mathbb{R}}_+$ be measures. If $\mu|_{\mathcal{G}} = \nu|_{\mathcal{G}}$ and \mathcal{G} contains a countable cover $(G_n)_{n \in \mathbb{N}}$ of X satisfying $\mu(G_n) = \nu(G_n) < \infty$ for all $n \in \mathbb{N}$ then $\mu = \nu$.

Theorem 4.1.4 (Extension Theorem for σ -finite Pre-Measures) Let X be a set, $\mathcal{S} \subseteq \mathcal{P}(X)$ be a semiring of sets and $\mu: \mathcal{S} \rightarrow \overline{\mathbb{R}}_+$ be a σ -finite pre-measure. Then there exists a uniquely determined measure $\hat{\mu}: \sigma_X(\mathcal{S}) \rightarrow \overline{\mathbb{R}}_+$ such that $\hat{\mu}|_{\mathcal{S}} = \mu$.

As we are only interested in finite measures, we provide a result, which can be derived easily from the identity theorem.

Corollary 4.1.5 (Equality of Finite Measures on Covering Semirings) Let X be an arbitrary set, $\mathcal{S} \subseteq \mathcal{P}(X)$ be a covering semiring and $\mu, \nu: \sigma_X(\mathcal{S}) \rightarrow \overline{\mathbb{R}}_+$ be finite measures. Then $\mu = \nu$ if and only if $\mu|_{\mathcal{S}} = \nu|_{\mathcal{S}}$.

Proof. Obviously we get $\mu|_{\mathcal{S}} = \nu|_{\mathcal{S}}$ if $\mu = \nu$. For the other direction let $(S_n)_{n \in \mathbb{N}}$ be a countable cover of X . Then finiteness of μ and ν together with the fact that measures are continuous (see above) and $\mu|_{\mathcal{S}} = \nu|_{\mathcal{S}}$ yield $\mu(S_n) = \nu(S_n) \leq$

$\nu(X) < \infty$ for all $n \in \mathbb{N}$. Since \mathcal{S} is a semiring of sets, it is closed under pairwise intersection which allows us to apply the identity theorem yielding $\mu = \nu$. \square

4.1.1 The Category of Measurable Spaces and Functions

Let X and Y be measurable spaces. A function $f: X \rightarrow Y$ is called *measurable* if and only if the pre-image of any measurable set of Y is a measurable set of X . The category Meas has measurable spaces as objects and measurable functions as arrows. Composition of arrows is function composition and the identity arrows are the identity functions.

The product of two measurable spaces (X, Σ_X) and (Y, Σ_Y) is the set $X \times Y$ endowed with the σ -algebra generated by $\Sigma_X * \Sigma_Y$, the set of so-called “rectangles” of measurable sets which is $\{S_X \times S_Y \mid S_X \in \Sigma_X, S_Y \in \Sigma_Y\}$. It is called the *product σ -algebra* of Σ_X and Σ_Y and is denoted by $\Sigma_X \otimes \Sigma_Y$. Whenever Σ_X and Σ_Y have suitable generators, we can also construct a possibly smaller generator for the product σ -algebra by taking only the “rectangles” of the generators.

Theorem 4.1.6 (Generators for the Product σ -Algebra) Let X, Y be arbitrary sets and $\mathcal{G}_X \subseteq \mathcal{P}(X), \mathcal{G}_Y \subseteq \mathcal{P}(Y)$ such that $X \in \mathcal{G}_X$ and $Y \in \mathcal{G}_Y$. Then the following holds:

$$\sigma_{X \times Y}(\mathcal{G}_X * \mathcal{G}_Y) = \sigma_X(\mathcal{G}_X) \otimes \sigma_Y(\mathcal{G}_Y).$$

A proof of this theorem can be found in many standard textbooks on measure theory [Els11]. We remark that there are (obvious) product endofunctors on the category of measurable spaces and functions.

Definition 4.1.7 (Product Functors) Let (Z, Σ_Z) be a measurable space. The endofunctor $Z \times _ : \text{Meas} \rightarrow \text{Meas}$ maps a measurable space (X, Σ_X) to the measurable space $(Z \times X, \Sigma_Z \otimes \Sigma_X)$ and a measurable function $f: X \rightarrow Y$ to the measurable function $Z \times f: Z \times X \rightarrow Z \times Y, (z, x) \mapsto (z, f(x))$. The functor $_ \times Z$ is constructed analogously.

The coproduct of two measurable spaces (X, Σ_X) and (Y, Σ_Y) is the set $X + Y$ endowed with $\Sigma_X \oplus \Sigma_Y := \{S_X + S_Y \mid S_X \in \Sigma_X, S_Y \in \Sigma_Y\}$ as σ -algebra, the *disjoint union σ -algebra*. Note that in contrast to the product no σ -operator is needed because $\Sigma_X \oplus \Sigma_Y$ itself is already a σ -algebra whereas $\Sigma_X * \Sigma_Y$ is usually not a σ -algebra. For generators of the disjoint union σ -algebra we provide and prove a comparable result to the one given above for the product σ -algebra.

Theorem 4.1.8 (Generators for the Disjoint Union σ -Algebra) Let X, Y be arbitrary sets and $\mathcal{G}_X \subseteq \mathcal{P}(X), \mathcal{G}_Y \subseteq \mathcal{P}(Y)$ such that $\emptyset \in \mathcal{G}_X$ and $Y \in \mathcal{G}_Y$. Then the

following holds:

$$\sigma_{X+Y}(\mathcal{G}_X \oplus \mathcal{G}_Y) = \sigma_X(\mathcal{G}_X) \oplus \sigma_Y(\mathcal{G}_Y). \quad (4.1.2)$$

In order to prove this, we cite another result from the literature [Els11, I.4.5 Korollar].

Lemma 4.1.9 Let X be an arbitrary set, $\mathcal{G} \subseteq \mathcal{P}(X)$ and $S \subseteq X$. Then $\sigma_S(\mathcal{G}|S) = \sigma_X(\mathcal{G})|S$ where $\mathcal{G}|S$ is the set $\{G \cap S \mid G \in \mathcal{G}\}$ and analogously $\sigma_X(\mathcal{G})|S$ is the set $\{G \cap S \mid G \in \sigma_X(\mathcal{G})\}$.

Proof of Theorem 4.1.8. Without loss of generality we assume that X and Y are disjoint. Hence for any subsets $A \subseteq X$, $B \subseteq Y$ we have $A \cap B = \emptyset$ and thus $A + B \cong A \cup B$. In order to prove Equation (4.1.2) we show both inclusions separately.

- \subseteq We have $\mathcal{G}_X \oplus \mathcal{G}_Y \subseteq \sigma_X(\mathcal{G}_X) \oplus \sigma_Y(\mathcal{G}_Y)$ and thus monotonicity and idempotence of the σ -operator immediately yield $\sigma_{X \cup Y}(\mathcal{G}_X \oplus \mathcal{G}_Y) \subseteq \sigma_X(\mathcal{G}_X) \oplus \sigma_Y(\mathcal{G}_Y)$.
- \supseteq Let $G \in \sigma_X(\mathcal{G}_X) \oplus \sigma_Y(\mathcal{G}_Y)$. Then $G = G_X \cup G_Y$ with $G_X \in \sigma_X(\mathcal{G}_X)$ and $G_Y \in \sigma_Y(\mathcal{G}_Y)$. We observe that $\mathcal{G}_X = (\mathcal{G}_X \oplus \mathcal{G}_Y)|X$ and by applying Lemma 4.1.9 we obtain that $\sigma_{X \cup Y}(\mathcal{G}_X \oplus \mathcal{G}_Y)|X = \sigma_X(\mathcal{G}_X)$. Thus there must be a $G'_Y \in \mathcal{P}(Y)$ such that $G_X \cup G'_Y \in \sigma_{X \cup Y}(\mathcal{G}_X \oplus \mathcal{G}_Y)$. Analogously there must be a $G'_X \in \mathcal{P}(X)$ such that $G'_X \cup G_Y \in \sigma_{X \cup Y}(\mathcal{G}_X \oplus \mathcal{G}_Y)$. We have $Y = \emptyset \cup Y \in \sigma_{X \cup Y}(\mathcal{G}_X \oplus \mathcal{G}_Y)$ and hence we also have $X = (X \cup Y) \setminus Y \in \sigma_{X \cup Y}(\mathcal{G}_X \oplus \mathcal{G}_Y)$. Thus we calculate

$$G = G_X \cup G_Y = ((G_X \cup G'_Y) \cap X) \cup ((G'_X \cup G_Y) \cap Y) \in \sigma_{X \cup Y}(\mathcal{G}_X \oplus \mathcal{G}_Y)$$

and hence can conclude that $\sigma_{X \cup Y}(\mathcal{G}_X \oplus \mathcal{G}_Y) \supseteq \sigma_X(\mathcal{G}_X) \oplus \sigma_Y(\mathcal{G}_Y)$. \square

As before we have endofunctors for the coproduct, the coproduct functors.

Definition 4.1.10 (Coproduct Functors) Let (Z, Σ_Z) be a measurable space. The endofunctor $_ + Z: \text{Meas} \rightarrow \text{Meas}$ maps a measurable space (X, Σ_X) to the measurable space $(X + Z, \Sigma_X \oplus \Sigma_Z)$ and a measurable function $f: X \rightarrow Y$ to the measurable function $f + Z: X + Z \rightarrow Y + Z$, $(x, 0) \mapsto (f(x), 0)$, $(z, 1) \mapsto (z, 1)$. The functor $Z + _: \text{Meas} \rightarrow \text{Meas}$ is constructed analogously.

For isomorphisms in Meas we provide the following characterization which we will need later for our main result.

Theorem 4.1.11 (Isomorphisms in Meas) Two measurable spaces X and Y are isomorphic in Meas if and only if there is a bijective function $\varphi: X \rightarrow Y$ such

that¹ $\varphi(\Sigma_X) = \Sigma_Y$. If Σ_X is generated by a set $\mathcal{S} \subseteq \mathcal{P}(X)$ then X and Y are isomorphic if and only if there is a bijective function $\varphi: X \rightarrow Y$ such that Σ_Y is generated by $\varphi(\mathcal{S})$. In this case \mathcal{S} is a (covering) semiring of sets [a σ -algebra] if and only if $\varphi(\mathcal{S})$ is a (covering) semiring of sets [a σ -algebra].

Again, we need a result from measure theory for the proof. This auxiliary result and its proof can be found in the referenced literature [Els11, I.4.4 Satz].

Lemma 4.1.12 Let X, Y be sets, $f: X \rightarrow Y$ be a function. Then for every subset $\mathcal{S} \subseteq \mathcal{P}(Y)$ it holds that $\sigma_X(f^{-1}(\mathcal{S})) = f^{-1}[\sigma_Y(\mathcal{S})]$.

Proof of Theorem 4.1.11. Since the identity arrows in Meas are the identity functions, we can immediately derive that any isomorphism $\varphi: X \rightarrow Y$ must be a bijective function. Measurability of φ and its inverse function $\varphi^{-1}: Y \rightarrow X$ yield $\varphi(\Sigma_X) = \Sigma_Y$. The equality $\sigma_Y(\varphi(\mathcal{S})) = \varphi(\sigma_X(\mathcal{S}))$ follows from Lemma 4.1.12 by taking $f = \varphi^{-1}$. The last equivalence is easy to verify using bijectivity of φ and φ^{-1} . \square

4.1.2 Borel-Sigma-Algebras and the Lebesgue Integral

Before we can define the probability and the subprobability monad, we give a crash course in (Lebesgue) integration² loosely based on standard textbooks [Ash72; Els11]. For that purpose let us fix a measurable space X and a measure μ on X . We want to integrate numerical functions $f: X \rightarrow \overline{\mathbb{R}}$ and in order to do that we need a suitable σ -algebra on $\overline{\mathbb{R}}$ to define measurability of such functions.

Recall that a topological space is a tuple (Y, \mathcal{T}) , where Y is a set and $\mathcal{T} \subseteq \mathcal{P}(Y)$ is a set containing the empty set, the set Y itself and is closed under arbitrary unions and finite intersections. The set \mathcal{T} is called the *topology* of Y and its elements are called *open sets*. The *Borel σ -algebra* on Y , denoted $\mathfrak{B}(Y)$, is the σ -algebra generated by the open sets \mathcal{T} of the topology, i.e., $\mathfrak{B}(Y) = \sigma_Y(\mathcal{T})$. Thus the Borel σ -algebra provides a connection of topological aspects and measurability. For the set of real numbers, it can be shown [Els11, I.4.3 Satz] that the Borel σ -algebra $\mathfrak{B}(\mathbb{R})$ is generated by the semiring of all left-open intervals

$$\mathfrak{B}(\mathbb{R}) = \sigma_{\mathbb{R}}(\{(a, b] \mid a, b \in \mathbb{R}, a \leq b\}).$$

¹For a set $\mathcal{S} \subseteq \mathcal{P}(X)$ and a function $\varphi: X \rightarrow Y$ we define $\varphi(\mathcal{S}) = \{\varphi(S_X) \mid S_X \in \mathcal{S}\} = \{\{\varphi(x) \mid x \in S_X\} \mid S_X \in \mathcal{S}\}$.

²For the purpose of this chapter, Riemann integration will not suffice but we will have to use the Lebesgue integral.

With this definition at hand, we now equip the set $\overline{\mathbb{R}}$ of extended reals with its Borel σ -algebra which can be defined as

$$\mathfrak{B}(\overline{\mathbb{R}}) = \sigma_{\overline{\mathbb{R}}}(\{B \cup E \mid B \in \mathfrak{B}(\mathbb{R}), E \subseteq \{-\infty, \infty\}\}).$$

A function $f: X \rightarrow \overline{\mathbb{R}}$ is called *(Borel-)measurable* if it is measurable with respect to this Borel σ -algebra. Given two Borel-measurable functions $f, g: Y \rightarrow \overline{\mathbb{R}}$ and real numbers α, β also $\alpha f + \beta g$ is Borel-measurable [Els11, Satz III.4.7] and thus are all finite linear combinations of Borel-measurable functions. Moreover, if $(f_n)_{n \in \mathbb{N}}$ is a sequence of Borel-measurable functions $f_n: X \rightarrow \overline{\mathbb{R}}$ converging pointwise to a function $f: X \rightarrow \overline{\mathbb{R}}$, then also f is Borel-measurable [Ash72, page 1.5.4]. In the remainder of this section we will just consider Borel-measurable functions.

We call f *simple* if and only if it attains only finitely many values, say $f(X) = \{\alpha_1, \dots, \alpha_N\}$. The integral of such a simple function f is then defined to be the μ -weighted sum of the α_n , formally $\int f d\mu = \sum_{n=1}^N \alpha_n \mu(S_n)$ where $S_n = f^{-1}[\alpha_n] \in \Sigma_X$ is measurable because $\{\alpha_n\}$ is measurable and f is a measurable function. Whenever f is non-negative we can approximate it from below using non-negative simple functions. In this case we define the integral to be

$$\int f d\mu := \sup \left\{ \int s d\mu \mid s \text{ non-negative and simple s.t. } 0 \leq s \leq f \right\}.$$

For arbitrary Borel-measurable f we decompose it into its positive part $f^+ := \max\{f, 0\}$ and negative part $f^- := \max\{-f, 0\}$ which are both non-negative and Borel-measurable. We note that $f = f^+ - f^-$ and consequently we define the integral of f to be the difference $\int f d\mu := \int f^+ d\mu - \int f^- d\mu$ if not both integrals on the right hand side are $+\infty$. In the latter case we say that the integral does not exist. Whenever it exists and is finite we call f a μ -*integrable function* or simply an *integrable function* if the measure μ is obvious from the context.

For every measurable set $S \in \Sigma_X$ its *characteristic function* $\chi_S: X \rightarrow \mathbb{R}$, which is 1 if $x \in S$ and 0 otherwise, is μ -integrable and for μ -integrable f the product $\chi_S \cdot f$ is also μ -integrable and we write

$$\int_S f d\mu := \int \chi_S \cdot f d\mu.$$

Instead of $\int_S f d\mu$ we will sometimes write $\int_S f(x) d\mu(x)$ or $\int_{x \in S} f(x) d\mu(x)$ which is useful if we have functions with more than one argument or multiple integrals. Note that this does not imply that singleton sets are measurable.

Some useful properties of the integral are that it is *linear*, i.e., for μ -integrable functions $f, g: X \rightarrow \overline{\mathbb{R}}$ and real numbers α, β we have

$$\int \alpha f + \beta g d\mu = \alpha \int f d\mu + \beta \int g d\mu$$

and the integral is *monotone*, i.e., $f \leq g$ implies $\int f d\mu \leq \int g d\mu$. We will state one result explicitly which we will use later in our proofs. This result and its proof can be found e.g. in [Ash72, Theorem 1.6.12].

Theorem 4.1.13 (Image Measure) Let X, Y be measurable spaces, μ be a measure on X , $f: Y \rightarrow \overline{\mathbb{R}}$ be a Borel-measurable function and $g: X \rightarrow Y$ be a measurable function. Then $\mu \circ g^{-1}$ is a measure³ on Y , the so-called *image-measure* and f is $(\mu \circ g^{-1})$ -integrable if and only if $f \circ g$ is μ -integrable and in this case we have $\int_S f d(\mu \circ g^{-1}) = \int_{g^{-1}[S]} f \circ g d\mu$ for all $S \in \Sigma_Y$.

4.1.3 The Probability and the Subprobability Monad

We will now introduce the probability monad (Giry monad) and the subprobability monad as presented in the literature [Gir82; Pan09]. First, we take a look at the endofunctors of these monads.

Definition 4.1.14 (The Subprobability and the Probability Functor) The *subprobability functor* $S: \text{Meas} \rightarrow \text{Meas}$ maps a measurable space (X, Σ_X) to the measurable space $(S(X), \Sigma_{S(X)})$ where $S(X)$ is the set of all subprobability measures on Σ_X and $\Sigma_{S(X)}$ is the smallest σ -algebra such that for all $S \in \Sigma_X$ the *evaluation maps*:

$$p_S: S(X) \rightarrow [0, 1], \quad p_S(P) = P(S) \quad (4.1.3)$$

are Borel-measurable. For any measurable function $f: X \rightarrow Y$ between measurable spaces $(X, \Sigma_X), (Y, \Sigma_Y)$ the arrow $S(f)$ maps a probability measure P to its image measure:

$$S(f): S(X) \rightarrow S(Y), \quad S(f)(P) := P \circ f^{-1}. \quad (4.1.4)$$

If we take full probabilities instead of sub-probabilities we get another endofunctor, the probability functor \mathbb{P} , analogously.

Both the subprobability functor S and the probability functor \mathbb{P} are functors of monads with the following unit and multiplication natural transformations.

Definition 4.1.15 (Unit and Multiplication) Let T be either the subprobability functor S or the probability functor \mathbb{P} . We obtain two natural transformations

³This notation is a bit lax. If we wanted to be really precise we would have to write $\mu \circ (g^{-1}|_{\Sigma_Y})$.

$\eta: \text{Id}_{\text{Meas}} \Rightarrow T$ and $\mu: T^2 \Rightarrow T$ by defining for every measurable space (X, Σ_X) :

$$\eta_X: X \rightarrow TX, \quad \eta_X(x) = \delta_x^X \quad (4.1.5)$$

$$\mu_X: T^2X \rightarrow TX, \quad \mu_X(P)(S) := \int p_S dP \quad \text{for } S \in \Sigma_X \quad (4.1.6)$$

where $\delta_x^X: \Sigma_X \rightarrow [0, 1]$ is the Dirac measure and p_S is the evaluation map (4.1.3) from above.

If we combine all the ingredients we obtain the following result which also guarantees the soundness of the previous definitions.

Theorem 4.1.16 ([Gir82; Pan09]) (S, η, μ) and (P, η, μ) are monads on Meas .

4.1.4 A Category of Stochastic Relations

The Kleisli category of the subprobability monad (S, η, μ) is sometimes called *category of stochastic relations* [Pan09] and denoted by SRel . Let us briefly analyze the arrows of this category: Given two measurable spaces (X, Σ_X) , (Y, Σ_Y) a Kleisli arrow $h: X \rightarrow SY$ maps each $x \in X$ to a subprobability measure $h(x): \Sigma_Y \rightarrow [0, 1]$. By uncurrying we can regard h as a function $h: X \times \Sigma_Y \rightarrow [0, 1]$. Certainly for each $x \in X$ the function $S \mapsto h(x, S)$ is a (sub)probability measure and one can show that for each $S \in \Sigma_Y$ the function $x \mapsto h(x, S)$ is Borel-measurable. Any function $h: X \times \Sigma_Y \rightarrow [0, 1]$ with these properties is called a *Markov kernel* or a *stochastic kernel* and it is known [Dob07a, Proposition 2.7] that these Markov kernels correspond exactly to the Kleisli arrows $h: X \rightarrow SY$.

We will later need the following, simple result about Borel-measurable functions and Markov kernels:

Lemma 4.1.17 Let (X, Σ_X) and (Y, Σ_Y) be measurable spaces, $g: Y \rightarrow [0, 1]$ be a Borel-measurable function and $h: X \times \Sigma_Y \rightarrow [0, 1]$ be a Markov kernel. Then the function $f: X \rightarrow [0, 1]$, $f(x) := \int_{y \in Y} g(y) dh(x, y)$ is Borel-measurable.

Proof. If g is a simple and Borel-measurable function, say $g(Y) = \{\alpha_1, \dots, \alpha_N\}$, then $f(x) = \sum_{n=1}^N \alpha_n h(x, A_n)$ where $A_n = g^{-1}[\{\alpha_n\}]$ and hence f is Borel-measurable as a linear combination of Borel-measurable functions. If g is an arbitrary, Borel-measurable function we approximate it from below with simple functions s_i , $i \in \mathbb{N}$ and define $f_i: X \rightarrow [0, 1]$ with $f_i(x) = \int_{y \in Y} s_i(y) dh(x, y)$. Then by the monotone convergence theorem [Ash72, page 1.6.2] we have

$$f(x) = \int_{y \in Y} \lim_{i \rightarrow \infty} s_i(y) dh(x, y) = \lim_{i \rightarrow \infty} f_i(x).$$

As shown before, each of the f_i is Borel-measurable and thus also the function f is Borel-measurable as pointwise limit of Borel-measurable functions. \square

4.2 Coalgebraic Probabilistic Traces

There is a big variety of probabilistic transition systems [Sok11; vGSST95]. We will deal with four slightly different versions of *generative* probabilistic transition system (PTS). The underlying intuition is that, according to a subprobability measure, an action from the alphabet A and a set of possible successor states are chosen. We distinguish between probabilistic branching according to subprobability and probability measures and furthermore we treat systems without and with termination.

Definition 4.2.1 (Continuous Probabilistic Transition System) A (continuous) *probabilistic transition system* (PTS) is a triple (A, X, α) where A is a finite alphabet (endowed with $\mathcal{P}(A)$ as σ -algebra), X is the *state space*, an arbitrary measurable space with σ -algebra Σ_X and α is the *transition function* which has one of the following forms and determines the type of the PTS.

Transition Function α	Type \diamond of the PTS
$\alpha: X \rightarrow \mathbb{S}(A \times X)$	0
$\alpha: X \rightarrow \mathbb{S}(A \times X + \mathbb{1})$	*
$\alpha: X \rightarrow \mathbb{P}(A \times X)$	ω
$\alpha: X \rightarrow \mathbb{P}(A \times X + \mathbb{1})$	∞

For every symbol $a \in A$ we define a Markov kernel $P_a: X \times \Sigma_X \rightarrow [0, 1]$ where

$$P_a(x, S) := \alpha(x)(\{a\} \times S). \quad (4.2.1)$$

Intuitively, $P_a(x, S)$ is the probability of making an a -transition from the state $x \in X$ to any state $y \in S$. Whenever X is a countable set and $\Sigma_X = \mathcal{P}(X)$ we call the PTS *discrete*. The unique state $\checkmark \in \mathbb{1}$ – whenever it is present – denotes termination of the system.

Note that we use the same abbreviation (PTS) as we have used in the Preliminaries for discrete systems modelled as coalgebras in *Set*. In this whole chapter we will always assume a PTS to be defined as above.

The reason for choosing the above symbols as type identifiers will only be revealed much later in Theorem 4.2.33 (page 118). In that theorem we will show that the coalgebraic traces of the respective systems are probability measures on the empty set $\emptyset = A^0$, the set A^* of all finite words, the set A^ω of all infinite words and the set A^∞ of all words.

Now we will first take a look at a small example PTS with type ∞ before we continue with our theory.

Example 4.2.2 (Discrete PTS with Finite and Infinite Traces) Let $A = \{a, b\}$, $X = \{0, 1, 2\}$, $\Sigma_X = \mathcal{P}(X)$ and $\alpha: X \rightarrow \mathbb{P}(A \times X + \mathbb{1})$ such that we obtain the system depicted in Figure 4.2.1.

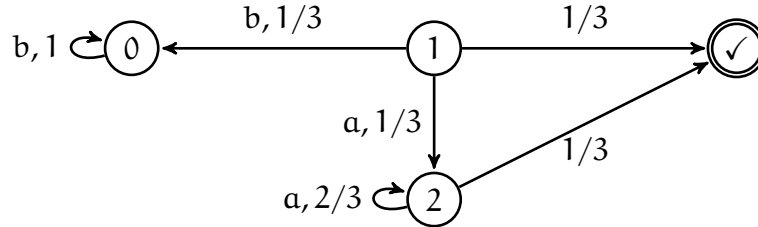


Figure 4.2.1: A discrete PTS

As stated in the definition, \checkmark is the unique final state. It has only incoming transitions bearing probabilities and no labels. These transitions describe the termination probability in the respective source state. For example, in state 1 the system terminates with probability $1/3$.

4.2.1 Towards Measurable Sets of Words: Cones and Semirings

In order to define a trace measure on these probabilistic transition systems we need suitable σ -algebras on the sets of words. While the set of all finite words, A^* , is rather simple – we will take $\mathcal{P}(A^*)$ as σ -algebra – the set of all infinite words, A^ω , and also the set of all finite and infinite words, A^∞ , needs some consideration. For a word $u \in A^*$ we call the set of all infinite words that have u as a prefix the ω -cone of u , denoted by uA^ω , and similarly we call the set of all finite and infinite words having u as a prefix the ∞ -cone [Pan09, p. 23] of u and denote it with uA^∞ . In the literature these sets are sometimes also-called “cylinder sets” [BKo8].

A cone can be visualized in the following way: For a given alphabet $A \neq \emptyset$ we consider the undirected, rooted and labelled tree given by $\mathcal{T} := (V, E, \varepsilon, l)$ with infinitely many vertices $V := A^*$, edges $E := \{\{u, ua\} \mid u \in A^*, a \in A\}$, root $\varepsilon \in A^*$ and edge-labeling function $l: E \rightarrow A, \{u, ua\} \mapsto a$. For $A = \{a, b, c\}$ the first three levels of the tree can be depicted as shown in Figure 4.2.2. Given a finite word $u \in A^*$, the ω -cone of u is represented by the set of all infinite paths⁴

⁴Within this chapter a path of an undirected graph (V, E) is always considered to be *simple*, i.e., any two vertices in a path are different.

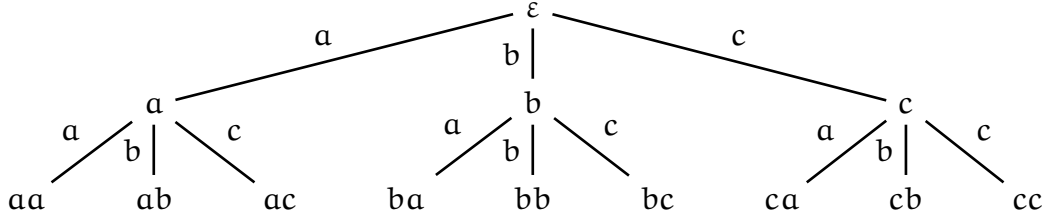


Figure 4.2.2: Visualization of Cones

that begin in ε and contain the vertex u and the ∞ -cone of u is represented by the set of all finite and infinite paths that begin in ε and contain the vertex u (and thus necessarily have a length which is greater or equal to the length of u).

Definition 4.2.3 (Cones of Words) Let A be a finite alphabet and let $\sqsubseteq \subset A^* \times A^\infty$ denote the usual prefix relation on words. For $u \in A^*$ we define its ω -cone to be the set $uA^\omega := \{v \in A^\omega \mid u \sqsubseteq v\}$ and analogously we define $uA^\infty := \{v \in A^\infty \mid u \sqsubseteq v\}$, the ∞ -cone of u .

With this definition at hand, we can now define the semirings we will use to generate σ -algebras on \emptyset , A^* , A^ω and A^∞ .

Definition 4.2.4 (Semirings of Sets of Words) Let A be a finite alphabet. We define

$$\begin{aligned} \mathcal{S}_0 &:= \{\emptyset\} \subset \mathcal{P}(\emptyset), \\ \mathcal{S}_* &:= \{\emptyset\} \cup \{\{u\} \mid u \in A^*\} \subset \mathcal{P}(A^*), \\ \mathcal{S}_\omega &:= \{\emptyset\} \cup \{uA^\omega \mid u \in A^*\} \subset \mathcal{P}(A^\omega), \\ \mathcal{S}_\infty &:= \{\emptyset\} \cup \{\{u\} \mid u \in A^*\} \cup \{uA^\infty \mid u \in A^*\} \subset \mathcal{P}(A^\infty). \end{aligned}$$

For the next theorem the fact that A is a finite alphabet is crucial.

Theorem 4.2.5 The sets \mathcal{S}_0 , \mathcal{S}_* , \mathcal{S}_ω and \mathcal{S}_∞ are covering semirings of sets.

Proof. For $\mathcal{S}_0 = \{\emptyset\}$ nothing has to be shown. Obviously we have $\emptyset \in \mathcal{S}_*$ and for elements $\{u\}, \{v\} \in \mathcal{S}_*$ we remark that $\{u\} \cap \{v\}$ is either $\{u\}$ if and only if $u = v$ or \emptyset else. Moreover, $\{u\} \setminus \{v\}$ is either \emptyset if and only if $u = v$ or $\{u\}$ else. We proceed with the proof for \mathcal{S}_∞ , the proof for \mathcal{S}_ω can be carried out almost analogously (in fact, it is simpler). By definition we have $\emptyset \in \mathcal{S}_\infty$. An intersection $uA^\infty \cap vA^\infty$ is non-empty if and only if either $u \sqsubseteq v$ or $v \sqsubseteq u$ and is then equal to vA^∞ or to uA^∞ and thus an element of \mathcal{S}_∞ . Similarly an intersection $uA^\infty \cap \{v\}$ is non-empty if and only if $u \sqsubseteq v$ and is then equal to $\{v\} \in \mathcal{S}_\infty$. As before we have

$\{u\} \cap \{v\} = \{u\}$ for $u = v$ and $\{u\} \cap \{v\} = \emptyset$ else. For the set difference $uA^\infty \setminus vA^\infty$ we note that this is either \emptyset (iff $v \sqsubseteq u$) or uA^∞ (iff $v \not\sqsubseteq u$ and $u \not\sqsubseteq v$) or otherwise ($u \sqsubseteq v$) the following union⁵ of finitely many disjoint sets in \mathcal{S}_∞ :

$$uA^\infty \setminus vA^\infty = \left(\bigcup_{v' \in A^{|v|} \setminus \{v\}, u \sqsubseteq v'} v'A^\infty \right) \cup \left(\bigcup_{v' \in A^{<|v|}, u \sqsubseteq v'} \{v'\} \right).$$

As before we get $\{u\} \setminus \{v\} = \emptyset$ if and only if $u = v$ and $\{u\} \setminus \{v\} = \{u\}$ else. For $\{u\} \setminus vA^\infty$ we observe that this is either $\{u\}$ if and only if $v \not\sqsubseteq u$ or \emptyset else. Finally, $uA^\infty \setminus \{v\}$ is either uA^∞ (iff $u \not\sqsubseteq v$) or ($u \sqsubseteq v$) the following union of finitely many disjoint sets in \mathcal{S}_∞ :

$$uA^\infty \setminus \{v\} = \left(\bigcup_{v' \in A^{|v|} \setminus \{v\}, u \sqsubseteq v'} v'A^\infty \right) \cup \left(\bigcup_{v' \in A^{<|v|}, u \sqsubseteq v'} \{v'\} \right) \cup \left(\bigcup_{a \in A} vaA^\infty \right)$$

which completes the proof that the given sets are semirings. The countable (and even disjoint) covers are: $\emptyset = \emptyset$, $A^* = \bigcup_{a \in A} \{a\}$, $A^\omega = \varepsilon A^\omega$ and $A^\infty = \varepsilon A^\infty$. \square

We remark that many interesting sets turn out to be measurable in the σ -algebra generated by the sets given in Definition 4.2.4. The singleton-set $\{u\}$ is measurable for every $u \in A^\omega$ because $\{u\} = \bigcap_{v \sqsubseteq u} vA^\omega = \bigcap_{v \sqsubseteq u} vA^\infty$ which are countable intersections, and (for ∞ -cones only) the set $A^* = \bigcup_{u \in A^*} \{u\}$ and consequently also the set $A^\omega = A^\infty \setminus A^*$ is measurable. The latter will be useful to check to what “extent” a state of a ∞ -PTS accepts finite or infinite behavior.

4.2.2 Measurable Sets of Words

Let us now take a closer look at the σ -algebras generated by the semirings which we defined in the last section. We obviously obtain the trivial σ -algebra $\sigma_\emptyset(\mathcal{S}_\emptyset) = \{\emptyset\}$. Since A is finite, A^* is countable and we can easily conclude $\sigma_{A^*}(\mathcal{S}_*) = \mathcal{P}(A^*)$. The other two cases need a more thorough treatment. For the remainder of this section let thus $\diamond \in \{\omega, \infty\}$. We will use the concepts of transfinite induction (as presented in the preliminaries) to extend the semi-ring \mathcal{S}_\diamond to the σ -algebra it generates. A similar construction is well-known and presented in the literature [Els11]. Usually this explicit construction is not needed but for our proofs it will turn out to be useful. An alternative proof technique for which this explicit construction is not needed can be found in Appendix A.2 .

⁵For $n \in \mathbb{N}$ we define $A^{<n} := \{u \in A \mid |u| < n\}$.

Definition 4.2.6 For any set X and $\mathcal{G} \subseteq \mathcal{P}X$ let $\mathcal{U}(\mathcal{G})$ and $\mathcal{I}(\mathcal{G})$ be the closure of \mathcal{G} under countable unions and intersections. We define

$$\begin{aligned}\mathcal{R}_\diamond(0) &:= \left\{ \bigcup_{n=1}^N S_n \mid N \in \mathbb{N}, S_n \in \mathcal{S}_\diamond \text{ disjoint} \right\}, \\ \mathcal{R}_\diamond(\alpha+1) &:= \mathcal{U}(\mathcal{I}(\mathcal{R}_\diamond(\alpha))) \quad \text{for every ordinal } \alpha \text{ and,} \\ \mathcal{R}_\diamond(\gamma) &:= \bigcup_{\alpha < \gamma} \mathcal{R}_\diamond(\alpha) \quad \text{for every limit ordinal } \gamma.\end{aligned}$$

Obviously we have $\mathcal{R}_\diamond(\alpha) \subseteq \mathcal{R}_\diamond(\beta)$ for all ordinals $\alpha < \beta$. Since \mathcal{S}_\diamond is a semiring of sets, is easy to see that $\mathcal{R}_\diamond(0)$ is an *algebra (of sets)*, i.e., it contains the base set A^\diamond , is closed under complement and binary (and hence all finite) unions and intersections.

Lemma 4.2.7 $S \in \mathcal{R}_\diamond(\gamma) \implies A^\diamond \setminus S \in \mathcal{R}_\diamond(\gamma)$ for every limit ordinal γ .

Proof. We will show that $S \in \mathcal{R}_\diamond(\alpha) \implies A^\diamond \setminus S \in \mathcal{I}(\mathcal{R}_\diamond(\alpha))$ for every ordinal α . This is true for the algebra $\mathcal{R}_\diamond(0)$. Now let α be an ordinal satisfying the implication and let $S \in \mathcal{R}_\diamond(\alpha+1)$. Then $S = \bigcup_{m=1}^\infty \bigcap_{n=1}^\infty S_{m,n}$ with $S_{m,n} \in \mathcal{R}_\diamond(\alpha)$ and by deMorgan's rules $A^\diamond \setminus S = \bigcap_{m=1}^\infty \bigcup_{n=1}^\infty A^\diamond \setminus S_{m,n}$ where by hypothesis $A^\diamond \setminus S_{m,n} \in \mathcal{I}(\mathcal{R}_\diamond(\alpha))$, thus $\bigcup_{n=1}^\infty A^\diamond \setminus S_{m,n} \in \mathcal{U}(\mathcal{I}(\mathcal{R}_\diamond(\alpha))) = \mathcal{R}_\diamond(\alpha+1)$ and therefore $A^\diamond \setminus S \in \mathcal{I}(\mathcal{R}_\diamond(\alpha+1))$. Finally, let γ be a limit ordinal and suppose the implication holds for all ordinals $\alpha < \gamma$. For any $S \in \mathcal{R}_\diamond(\gamma)$ there is an $\alpha < \gamma$ such that $S \in \mathcal{R}_\diamond(\alpha)$. Hence we have $A^\diamond \setminus S \in \mathcal{I}(\mathcal{R}_\diamond(\alpha)) \subseteq \mathcal{R}_\diamond(\alpha+1) \subseteq \mathcal{R}_\diamond(\gamma)$. \square

Lemma 4.2.8 $S, T \in \mathcal{R}_\diamond(\alpha) \implies S \cup T, S \cap T \in \mathcal{R}_\diamond(\alpha)$ for every ordinal α .

Proof. This is true for the algebra $\mathcal{R}_\diamond(0)$. Let α be an ordinal satisfying the implication and $S, T \in \mathcal{R}_\diamond(\alpha+1)$, then $S = \bigcup_{k=1}^\infty \bigcap_{l=1}^\infty S_{k,l}$ and $T = \bigcup_{m=1}^\infty \bigcap_{n=1}^\infty T_{m,n}$ with $S_{k,l}, T_{m,n} \in \mathcal{R}_\diamond(\alpha)$. Obviously $S \cup T = \bigcup_{k,m=1}^\infty \bigcap_{l,n=1}^\infty (S_{k,l} \cup T_{m,n})$ and $S \cap T = \bigcup_{k,m=1}^\infty \bigcap_{l,n=1}^\infty (S_{k,l} \cap T_{m,n})$ where by hypothesis $S_{k,l} \cup T_{m,n}, S_{k,l} \cap T_{m,n} \in \mathcal{R}_\diamond(\alpha)$ and thus $S \cup T, S \cap T \in \mathcal{R}_\diamond(\alpha+1)$. Finally, let γ be a limit ordinal and suppose the statement is true for all ordinals $\alpha < \gamma$ and let $S, T \in \mathcal{R}_\diamond(\gamma)$. There must be ordinals $\alpha, \beta < \gamma$ such that $S \in \mathcal{R}_\diamond(\alpha)$ and $T \in \mathcal{R}_\diamond(\beta)$. Without loss of generality we assume $\alpha \leq \beta$ then, since $\mathcal{R}_\diamond(\alpha) \subseteq \mathcal{R}_\diamond(\beta)$ we have $S \in \mathcal{R}_\diamond(\beta)$, hence $S \cup T, S \cap T \in \mathcal{R}_\diamond(\beta) \subseteq \mathcal{R}_\diamond(\gamma)$ which completes the proof. \square

Lemma 4.2.9 $S, T \in \mathcal{I}(\mathcal{R}_\diamond(\alpha)) \implies S \cup T \in \mathcal{I}(\mathcal{R}_\diamond(\alpha))$ for every ordinal α .

Proof. Let $S, T \in \mathcal{I}(\mathcal{R}_\diamond(\alpha))$ then $S := \bigcap_{m=1}^\infty S_m$ and $T := \bigcap_{n=1}^\infty T_n$ with $S_m, T_n \in \mathcal{R}_\diamond(\alpha)$. Then $S \cup T = \bigcap_{m,n=1}^\infty (S_m \cup T_n)$ where $S_m \cup T_n \in \mathcal{R}_\diamond(\alpha)$ by Lemma 4.2.8 and thus $S \cup T \in \mathcal{I}(\mathcal{R}_\diamond(\alpha))$. \square

Theorem 4.2.10 (Explicit Construction of the Generated Sigma-Algebra) Let ω_1 be the smallest uncountable limit ordinal then $\sigma_{A^\diamond}(\mathcal{S}_\diamond) = \sigma_{A^\diamond}(\mathcal{R}_\diamond(0)) = \mathcal{R}_\diamond(\omega_1)$.

Proof (adapted from [Els11]). By definition of the set $\mathcal{R}_\diamond(0)$ we have the inclusions $\mathcal{S}_\diamond \subseteq \mathcal{R}_\diamond(0) \subseteq \sigma_{A^\diamond}(\mathcal{S}_\diamond)$. Using the monotonicity of the σ -operator, we conclude that $\sigma_{A^\diamond}(\mathcal{S}_\diamond) \subseteq \sigma_{A^\diamond}(\mathcal{R}_\diamond(0)) \subseteq \sigma_{A^\diamond}(\mathcal{S}_\diamond)$ so all of them must be equal.

For the second equality we first show $\mathcal{R}_\diamond(\omega_1) \subseteq \sigma_X(\mathcal{R}_\diamond(0))$. We know that $\mathcal{R}_\diamond(0) \subseteq \sigma_X(\mathcal{R}_\diamond(0))$. For an ordinal α with $\mathcal{R}_\diamond(\alpha) \subseteq \sigma_X(\mathcal{R}_\diamond(0))$ let $S \in \mathcal{R}_\diamond(\alpha + 1)$. Then $S = \bigcup_{m=1}^{\infty} \bigcap_{n=1}^{\infty} S_{m,n}$ with $S_{m,n} \in \mathcal{R}_\diamond(\alpha)$ yielding $S \in \sigma_X(\mathcal{R}_\diamond(0))$. If γ is a limit ordinal with $\mathcal{R}_\diamond(\alpha) \subseteq \sigma_X(\mathcal{R}_\diamond(0))$ for all ordinals $\alpha < \gamma$ then for any $S \in \mathcal{R}_\diamond(\gamma)$ there must be an ordinal $\alpha < \gamma$ such that $S \in \mathcal{R}_\diamond(\alpha)$ and hence $S \in \sigma_X(\mathcal{R}_\diamond(0))$. In order to show $\mathcal{R}_\diamond(\omega_1) \supseteq \sigma_X(\mathcal{R}_\diamond(0))$ it suffices to show that $\mathcal{R}_\diamond(\omega_1)$ is a σ -algebra. We have $X \in \mathcal{R}(0) \subseteq \mathcal{R}(\omega_1)$ and Lemma 4.2.7 yields closure under complements. Let $S_n \in \mathcal{R}_\diamond(\omega_1)$ for $n \in \mathbb{N}$. Then for each S_n we have an α_n such that $S_n \in \mathcal{R}_\diamond(\alpha_n)$. Since ω_1 is the first uncountable ordinal, we must find an $\alpha < \omega_1$ such that $\alpha_n < \alpha$ for all $n \in \mathbb{N}$. Hence we have $S_n \in \mathcal{R}_\diamond(\alpha)$ for all $n \in \mathbb{N}$. Thus $\bigcup_{n=1}^{\infty} S_n \in \mathcal{R}_\diamond(\alpha + 1) \subseteq \mathcal{R}_\diamond(\omega_1)$. \square

4.2.3 The Trace Measure

We will now define the trace measure which can be understood as the behavior of a state: it measures the probability of accepting a set of words. Later we will prove that this can be captured by the unique map into a final coalgebra in the Kleisli category of the probability/probability monad.

Definition 4.2.11 (The Trace Measure) Let (A, X, α) be a \diamond -PTS. For every state $x \in X$ we define the trace (sub)probability measure $\text{tr}(x): \sigma_{A^\diamond}(\mathcal{S}_\diamond) \rightarrow [0, 1]$ as follows: In all four cases we require $\text{tr}(x)(\emptyset) = 0$. For $\diamond \in \{*, \infty\}$ we define

$$\text{tr}(x)(\{\varepsilon\}) = \alpha(x)(\mathbb{1}) \quad (4.2.2)$$

and

$$\text{tr}(x)(\{au\}) := \int_{x' \in X} \text{tr}(x')(\{u\}) dP_a(x, x') \quad (4.2.3)$$

for all $a \in A$ and all $u \in A^*$. For $\diamond \in \{\omega, \infty\}$ we define

$$\text{tr}(x)(A^\diamond) = 1 \quad (4.2.4)$$

and

$$\text{tr}(x)(auA^\diamond) := \int_{x' \in X} \text{tr}(x')(uA^\diamond) dP_a(x, x') \quad (4.2.5)$$

for all $a \in A$ and all $u \in A^*$.

We need to verify that everything is well-defined and sound. In the next theorem we explicitly state what has to be shown.

Theorem 4.2.12 For all four types $\diamond \in \{0, *, \omega, \infty\}$ of PTS the equations in Definition 4.2.11 yield a σ -finite pre-measure $\text{tr}(x): \mathcal{S}_\diamond \rightarrow [0, 1]$ for every $x \in X$. Moreover, the unique extension of this pre-measure is a (sub)probability measure.

Before we prove this theorem, let us try to get a more intuitive understanding of Definition 4.2.11 and especially equation (4.2.3). First we check how the above definition reduces when we consider discrete systems.

Remark 4.2.13 Let (A, X, α) be a discrete⁶ $*$ -PTS, i.e., X is a countable set with σ -algebra $\mathcal{P}(X)$ and the transition probability function is $\alpha: X \rightarrow \mathcal{S}(A \times X + \mathbb{1})$. Then $\text{tr}(x)(\varepsilon) := \alpha(x)(\checkmark)$ and (4.2.3) is equivalent to

$$\text{tr}(x)(au) := \sum_{x' \in X} \text{tr}(x')(u) \cdot P_a(x, x') \quad (4.2.6)$$

for all $a \in A$ and all $u \in A^*$ which in turn is equivalent to the discrete trace distribution for the sub-distribution monad \mathcal{D} on Set [HJS06].

Having seen this coincidence with known results, we proceed to calculate the trace measure for our example (Example 4.2.2) which we can only do in our more general setting because this ∞ -PTS is a discrete probabilistic transition system which exhibits both finite and infinite behavior.

Example 4.2.14 (Example 4.2.2 continued) We calculate the trace measures for the ∞ -PTS from Example 4.2.2 (page 98) and claim that $\text{tr}(0) = \delta_{b^\omega}^{A^\infty}$. First of all we show by induction that $\text{tr}(0)(b^k A^\infty) = 1$ holds. This is immediate for $k = 0$ by equation (4.2.4) of Definition 4.2.11. If we assume that our hypothesis holds for a given $k \in \mathbb{N}$, we can use the fact that in our example $P_b(0, _) = \delta_0^X$ and thus by equation (4.2.5) of Definition 4.2.11 we have $\text{tr}(0)(b^{k+1} A^\infty) = \text{tr}(0)(bb^k A^\infty) = \int_{x' \in X} \text{tr}(x')(b^k A^\infty) dP_b(0, x') = \text{tr}(0)(b^k A^\infty) = 1$. With this preparation at hand we compute

$$\text{tr}(0)(\{b^\omega\}) = \text{tr}(0)\left(\bigcap_{k=0}^{\infty} b^k A^\infty\right) = \text{tr}(0)\left(A^\infty \setminus \bigcup_{k=0}^{\infty} (A^\infty \setminus b^k A^\infty)\right)$$

⁶If Z is a countable set and $\mu: \mathcal{P}(Z) \rightarrow [0, 1]$ is a measure, we write $\mu(z)$ for $\mu(\{z\})$.

$$\begin{aligned}
 &= \text{tr}(0)(A^\infty) - \text{tr}(0)\left(\bigcup_{k=0}^{\infty} (A^\infty \setminus b^k A^\infty)\right) \\
 &\geq 1 - \sum_{k=0}^{\infty} \text{tr}(0)(A^\infty \setminus b^k A^\infty) \\
 &= 1 - \sum_{k=0}^{\infty} (1 - \text{tr}(0)(b^k A^\infty)) = 1 - \sum_{k=0}^{\infty} (1 - 1) = 1.
 \end{aligned}$$

Thus we have $\text{tr}(0) = \delta_{b^\omega}^{A^\infty}$ and therefore $\text{tr}(0)(A^*) = \text{tr}(0)(\bigcup_{u \in A^*} \{u\}) = 0$ and $\text{tr}(0)(A^\omega) = 1$. Again by induction we can show that $\text{tr}(2)(\{a^k\}) = (1/3) \cdot (2/3)^k$ and thus $\text{tr}(2)(A^*) = 1$ because

$$1 \geq \text{tr}(2)(A^*) = \text{tr}(2)\left(\bigcup_{u \in A^*} \{u\}\right) \geq \text{tr}(2)\left(\bigcup_{k=0}^{\infty} \{a^k\}\right) = \frac{1}{3} \cdot \sum_{k=0}^{\infty} \left(\frac{2}{3}\right)^k = 1$$

and hence we conclude $\text{tr}(2)(A^\omega) = 0$. Furthermore we calculate $\text{tr}(1)(\{b^\omega\}) = 1/3$, $\text{tr}(1)(aA^\infty) = 1/3$ and $\text{tr}(1)(\{\varepsilon\}) = 1/3$ yielding $\text{tr}(1)(A^*) = 2/3$ and $\text{tr}(1)(A^\omega) = 1/3$.

After this small example, we remember that we still have to prove Theorem 4.2.12. In order to simplify this proof, we provide a few technical results about the sets \mathcal{S}_* , \mathcal{S}_ω , \mathcal{S}_∞ . For all these results remember again that A is required to be a *finite* alphabet. This is a crucial point, particularly in the next lemma.

Lemma 4.2.15 (Countable Unions) Let $(S_n)_{n \in \mathbb{N}}$ be a sequence of pairwise disjoint sets in \mathcal{S}_ω or in \mathcal{S}_∞ such that their union, $\bigcup_{n \in \mathbb{N}} S_n$, is itself an element of \mathcal{S}_ω or \mathcal{S}_∞ . Then $S_n = \emptyset$ for all but finitely many n .

Proof. We have several cases to consider.

Case 1: If $\bigcup_{n \in \mathbb{N}} S_n = \emptyset \in \mathcal{S}_\diamond$ for $\diamond \in \{\omega, \infty\}$, we have $S_n = \emptyset$ for all $n \in \mathbb{N}$.

Case 2: If $\bigcup_{n \in \mathbb{N}} S_n = \{u\} \in \mathcal{S}_\infty$ with suitable $u \in A^*$ we get $S_n = \emptyset$ for all but one $n \in \mathbb{N}$ since the S_n are disjoint.

Case 3: Let $\bigcup_{n \in \mathbb{N}} S_n = uA^\diamond$ with a suitable $u \in A^*$ for $\diamond \in \{\omega, \infty\}$. Suppose there are infinitely many $n \in \mathbb{N}$ such that $S_n \neq \emptyset$. Without loss of generality we can assume $S_n \neq \emptyset$ for all $n \in \mathbb{N}$ and thus there is an infinite set $U := \{u_n \mid n \in \mathbb{N}\}$ of words such that for each $n \in \mathbb{N}$ we either have $S_n = \{u_n\}$ (only for $\diamond = \infty$) or $S_n = u_n A^\diamond$ (for $\diamond \in \{\omega, \infty\}$). Necessarily we have $u \sqsubseteq u_n$ for all $n \in \mathbb{N}$. We will now revive our tree metaphor from Section 4.2.1: The prefix-closure $\text{pref}(U) = \{v \in A^* \mid \exists n \in \mathbb{N} : v \sqsubseteq u_n\}$ of U is the set of vertices contained in the paths from the root ε (via u) to u_n . We consider the subtree $\mathcal{T}' = (\text{pref}(U), E', \varepsilon, \upharpoonright_{E'})$ with

$E' = \{\{u, ua\} \mid a \in A, u, ua \in \text{pref}(U)\}$. Since the set U and hence also $\text{pref}(U)$ is infinite, we have thus constructed an infinite, connected graph where every vertex has finite degree (because A is finite). By König's Lemma [Kon36, Satz 3] there is an infinite path starting at the root ε . Let $v \in A^\omega$ be the unique, infinite word associated to that path (which we get by concatenating all the labels along this path). Since $u \sqsubset v$ we must have $v \in uA^\diamond$. Moreover, we know that $uA^\diamond = \bigcup_{n \in \mathbb{N}} S_n$ and due to the fact that the S_n are pairwise disjoint we must find a unique $m \in \mathbb{N}$ with $v \in S_m$. This necessarily requires S_m to be a cone of the form $S_m = u_m A^\diamond$ with $u_m \in U$ and $u_m \sqsubset v$. Again due to the fact that the S_n are disjoint we know that there cannot be a $u' \in U$ with $u_m \sqsubset u'$ and hence there also cannot be a $u' \in \text{pref}(U)$ with $u_m \sqsubset u'$. Thus the vertex u_m is a leaf of the tree \mathcal{T}' and therefore the finite path from ε to u_m is the only path from ε that contains u_m . This contradicts the existence of v because this path is infinite and contains u_m . Hence our assumption must have been wrong and there cannot be infinitely many $n \in \mathbb{N}$ with $S_n \neq \emptyset$. \square

Lemma 4.2.16 Any map $\mu: \mathcal{S}_* \rightarrow \overline{\mathbb{R}}_+$ where $\mu(\emptyset) = 0$ is σ -additive and thus a pre-measure.

Proof. Let $(S_n)_{n \in \mathbb{N}}$ be a family of disjoint sets from \mathcal{S}_* with $(\bigcup_{n \in \mathbb{N}} S_n) \in \mathcal{S}_*$, then we have $S_n = \emptyset$ for all but at most one $n \in \mathbb{N}$. \square

Lemma 4.2.17 A map $\mu: \mathcal{S}_\omega \rightarrow \overline{\mathbb{R}}_+$ where $\mu(\emptyset) = 0$ is σ -additive and thus a pre-measure if and only if the following equation holds for all $u \in A^*$.

$$\mu(uA^\omega) = \sum_{a \in A} \mu(uaA^\omega) \quad (4.2.7)$$

We omit the proof of this lemma as it is very similar to the proof of the following lemma.

Lemma 4.2.18 A map $\mu: \mathcal{S}_\infty \rightarrow \overline{\mathbb{R}}_+$ where $\mu(\emptyset) = 0$ is σ -additive and thus a pre-measure if and only if the following equation holds for all $u \in A^*$.

$$\mu(uA^\infty) = \mu(\{u\}) + \sum_{a \in A} \mu(uaA^\infty) \quad (4.2.8)$$

Proof. Obviously σ -additivity of μ implies equality (4.2.8). Let now $(S_n)_{n \in \mathbb{N}}$ be a family of disjoint sets from \mathcal{S}_∞ with $(\bigcup_{n \in \mathbb{N}} S_n) \in \mathcal{S}_\infty$. Using Lemma 4.2.15 we know that we can assume that there is an $N \in \mathbb{N}$ such that $S_n \neq \emptyset$ for $1 \leq n \leq N$ and $S_n = \emptyset$ for $n > N$. For non-trivial cases (trivial means $S_n = \emptyset$ for all but one set) there must be a word $u \in A^*$ such that $uA^\infty = (\bigcup_{n=1}^N S_n)$. Because u is

an element of uA^∞ there must be a natural number m with $u \in S_m$ which is unique because the family is disjoint. Without loss of generality we assume that $u \in S_1$. By construction of \mathcal{S}_∞ and the fact that $\bigcup_{n=1}^N S_n = uA^\infty$ there are two cases to consider: either $S_1 = \{u\}$ or $S_1 = uA^\infty$. The latter cannot be true since this would imply $S_n = \emptyset$ for $n \geq 2$ which we explicitly excluded. Thus we have $S_1 = \{u\}$. We remark that

$$\bigcup_{a \in A} uaA^\infty = uA^\infty \setminus \{u\} = \left(\bigcup_{n=2}^N S_n \right).$$

Again by construction of \mathcal{S}_∞ we must be able to select sets $S_k^a \in \{S_n \mid 2 \leq n \leq N\}$ for all $a \in A$ and all k where $1 \leq k \leq K_a < N$ for a constant K_a such that $\bigcup_{k=1}^{K_a} S_k^a = uaA^\infty$. This selection is unique in the following manner: For $a, b \in A$ where $a \neq b$ and $1 \leq k \leq K_a, 1 \leq l \leq K_b$ we have $S_k^a \neq S_l^b$. Additionally it is complete in the sense that $\{S_k^a \mid a \in A, 1 \leq k \leq K_a\} = \{S_n \mid 2 \leq n \leq N\}$. We apply our equation (4.2.8) to get

$$\mu \left(\bigcup_{n=1}^N S_n \right) = \mu(uA^\infty) = \mu(S_1) + \sum_{a \in A} \mu \left(\bigcup_{k=1}^{K_a} S_k^a \right)$$

and note that we can repeat the procedure for each of the disjoint unions $\bigcup_{k=1}^{K_a} S_k^a$. Since $K_a < N$ for all a this procedure stops after finitely many steps yielding σ -additivity of μ . \square

Using these results, we can now finally prove Theorem 4.2.12.

Proof of Theorem 4.2.12. We will look at the different types of PTS separately. For $\diamond = 0$ nothing has to be shown because $\sigma_\emptyset(\{\emptyset\}) = \{\emptyset\}$ and $\text{tr}(x): \{\emptyset\} \rightarrow [0, 1]$ is already uniquely defined by $\text{tr}(x)(\emptyset) = 0$. For $\diamond = *$ Lemma 4.2.16 yields immediately that the equations define a pre-measure. For $\diamond = \infty$ we have to check validity of equation (4.2.8) of Lemma 4.2.18. We will do so using induction on the length of the word $u \in A^*$ in that equation. We have

$$\begin{aligned} \text{tr}(x)(\varepsilon A^\infty) &= 1 = \alpha(x)(A \times X + \mathbb{1}) = \alpha(x)(\mathbb{1}) + \sum_{a \in A} P_a(x, X) \\ &= \text{tr}(x)(\{\varepsilon\}) + \sum_{a \in A} \int_{x' \in X} 1 \, dP_a(x, x') \\ &= \text{tr}(x)(\{\varepsilon\}) + \sum_{a \in A} \int_{x' \in X} \text{tr}(x')(\varepsilon A^\infty) \, dP_a(x, x') \\ &= \text{tr}(x)(\{\varepsilon\}) + \sum_{a \in A} \text{tr}(x)(a\varepsilon A^\infty) = \text{tr}(x)(\{\varepsilon\}) + \sum_{a \in A} \text{tr}(x)(\varepsilon aA^\infty) \end{aligned}$$

for all $x \in X$. Now let us assume that for all $x \in X$ and all words $u \in A^{\leq n}$ of length less or equal to a fixed $n \in \mathbb{N}$ the induction hypothesis

$$\text{tr}(x)(uA^\infty) = \text{tr}(x)(\{u\}) + \sum_{b \in A} \text{tr}(x)(ubA^\infty)$$

is fulfilled. Then for all $x \in X$, all $a \in A$ and all $u \in A^{\leq n}$ we calculate

$$\begin{aligned} \text{tr}(x)(auA^\infty) &= \int_{x' \in X} \text{tr}(x')(uA^\infty) dP_a(x, x') \\ &= \int_{x' \in X} \left(\text{tr}(x')(\{u\}) + \sum_{b \in A} \text{tr}(x')(ubA^\infty) \right) dP_a(x, x') \\ &= \int_{x' \in X} \text{tr}(x')(\{u\}) dP_a(x, x') + \sum_{b \in A} \int_{x' \in X} \text{tr}(x')(ubA^\infty) dP_a(x, x') \\ &= \text{tr}(x)(\{au\}) + \sum_{b \in A} \text{tr}(x)(aubA^\infty) \end{aligned}$$

and hence also for $au \in A^{\leq n+1}$ equation (4.2.8) is fulfilled and by induction we conclude that it is valid for all $u \in A^*$. The only difficult case is $\diamond = \omega$ where we will, of course, apply Lemma 4.2.17. Let $u = u_1 \dots u_m$ with $u_k \in A$ for every $k \in \mathbb{N}$ with $k \leq m$, then multiple application of the defining equation (4.2.3) yields

$$\text{tr}(x)(uA^\omega) = \int_{x_1 \in X} \dots \int_{x_m \in X} 1 dP_{u_m}(x_{m-1}, x_m) \dots dP_{u_1}(x, x_1)$$

and for arbitrary $a \in A$ we obtain analogously:

$$\text{tr}(x)(uaA^\omega) = \int_{x_1 \in X} \dots \int_{x_m \in X} P_a(x_m, X) dP_{u_m}(x_{m-1}, x_m) \dots dP_{u_1}(x, x_1).$$

All integrals exist and are bounded above by 1 so we can use the linearity and monotonicity of the integral to exchange the finite sum and the integrals. Using the fact that

$$\sum_{a \in A} P_a(x_m, X) = \sum_{a \in A} \alpha(x_m)(\{a\} \times X) = \alpha(x_m)(A \times X) = 1$$

we obtain that indeed the necessary and sufficient equality

$$\text{tr}(x)(uA^\omega) = \sum_{a \in A} \text{tr}(x)(uaA^\omega)$$

is valid for all $u \in A^*$ and thus Lemma 4.2.17 yields that also $\text{tr}(x): \mathcal{S}_\omega \rightarrow \overline{\mathbb{R}}_+$ is σ -additive and thus a pre-measure.

Now let us check that the pre-measures for $\diamond \in \{*, \omega, \infty\}$ are σ -finite and that their unique extensions are (sub)probability measures. For $\diamond \in \{\omega, \infty\}$ this is obvious and in these cases the unique extension must be a probability measure because by definition we have $\text{tr}(x)(A^\omega) = 1$ and $\text{tr}(x)(A^\infty) = 1$ respectively. For the remaining case ($\diamond = *$) we will use induction. We have $\text{tr}(x)(\{\varepsilon\}) = \alpha(x)(\mathbb{1}) \leq 1$ for every $x \in X$. Let us now assume that for a fixed but arbitrary $n \in \mathbb{N}$ the inequality $\text{tr}(x)(\{u\}) \leq 1$ is valid for all $x \in X$ and all words $u \in A^{\leq n}$ with length less or equal to n . Then for any word $u' \in A^{n+1}$ of length $n+1$ we have $u' = au$ with $a \in A$ and $u \in A^n$. We observe that

$$\text{tr}(x)(\{au\}) = \int_{x' \in X} \underbrace{\text{tr}(x')(\{u\})}_{\leq 1} dP_a(x, x') \leq \int 1 dP_a(x, x') = P_a(x, X) \leq 1$$

and conclude by induction that $\text{tr}(x)(\{u\}) \leq 1$ is valid for all $u \in A^*$ and all $x \in X$. Due to the fact that $A^* = \bigcup_{u \in A^*} \{u\}$ this yields that tr is σ -finite.

Again by induction we will show that tr is bounded above by 1 and thus a subprobability measure. We have $\text{tr}(x)(A^{\leq 0}) = \text{tr}(x)(\{\varepsilon\}) \leq 1$ for all $x \in X$. Suppose that for a fixed but arbitrary $n \in \mathbb{N}$ the inequality $\text{tr}(x)(A^{\leq n-1}) \leq 1$ holds for all $x \in X$. We conclude with the following calculation

$$\begin{aligned} \text{tr}(x)(A^{\leq n}) &= \text{tr}(x)\left(\bigcup_{u \in A^{\leq n}} \{u\}\right) = \sum_{u \in A^{\leq n}} \text{tr}(x)(\{u\}) \\ &= \text{tr}(x)(\{\varepsilon\}) + \sum_{a \in A} \sum_{u \in A^{\leq n-1}} \text{tr}(x)(\{au\}) \\ &= \alpha(x)(\mathbb{1}) + \sum_{a \in A} \sum_{u \in A^{\leq n-1}} \int \text{tr}(x')(\{u\}) dP_a(x, x') \\ &= \alpha(x)(\mathbb{1}) + \sum_{a \in A} \int \sum_{u \in A^{\leq n-1}} \text{tr}(x')(\{u\}) dP_a(x, x') \\ &= \alpha(x)(\mathbb{1}) + \sum_{a \in A} \int \underbrace{\left(\text{tr}(x')(A^{\leq n-1})\right)}_{\leq 1} dP_a(x, x') \\ &\leq \alpha(x)(\mathbb{1}) + \sum_{a \in A} \int 1 dP_a(x, x') = \alpha(x)(\mathbb{1}) + \sum_{a \in A} P_a(x, X) \\ &= \alpha(x)(\mathbb{1}) + \sum_{a \in A} \alpha(x)(\{a\} \times X) = \alpha(x)(A \times X + \mathbb{1}) \leq 1 \end{aligned}$$

using the linearity and monotonicity of the integral which can be applied here since A is finite which in turn implies that $A^{\leq n-1}$ is finite and all the integrals

$\int \text{tr}(x')(\{u\}) dP_a(x, x')$ exist because $\text{tr}(x')(\{u\})$ is bounded above by 1. By induction we can thus conclude that

$$\forall x \in X \forall n \in \mathbb{N}_0 : \text{tr}(x)(A^{\leq n}) \leq 1$$

which is equivalent to

$$\forall x \in X \sup_{n \in \mathbb{N}_0} (\text{tr}(x)(A^{\leq n})) \leq 1.$$

Since $\text{tr}(x)$ is a measure (and thus non-negative and σ -additive), the sequence given by $(\text{tr}(x)(A^{\leq n}))_{n \in \mathbb{N}_0}$ is a monotonically increasing sequence of real numbers bounded above by 1. Furthermore, $\text{tr}(x)$ is continuous from below as a measure and we have $A^{\leq n} \subseteq A^{\leq n+1}$ for all $n \in \mathbb{N}_0$ and thus we obtain

$$\text{tr}(x)(A^*) = \text{tr}(x)\left(\bigcup_{n=1}^{\infty} A^{\leq n}\right) = \lim_{n \rightarrow \infty} \text{tr}(x)(A^{\leq n}) = \sup_{n \in \mathbb{N}_0} \text{tr}(x)(A^{\leq n}) \leq 1.$$

□

4.2.4 The Trace Function is a Kleisli Arrow

Now that we know that our definition of a trace measure is mathematically sound, we remember that we wanted to show that it is “natural”, meaning that it arises from the final coalgebra in the Kleisli category of the (sub)probability monad.

We start by showing that the function $\text{tr}: X \rightarrow TA^\diamond$ we get from Definition 4.2.11 is a Kleisli arrow by proving that it is a Markov kernel. Since $\text{tr}(x)$ is a subprobability measure for each $x \in X$ by Theorem 4.2.12 we just have to show that for each $S \in \sigma_{A^\diamond}(\mathcal{S}_\diamond)$ the function $x \mapsto \text{tr}(x)(S)$ is Borel-measurable. This is easy for elements S of the previously defined semirings:

Lemma 4.2.19 For all $S \in \mathcal{S}_\diamond$ the function $x \mapsto \text{tr}(x)(S)$ is measurable.

Proof. For $\diamond = 0$ nothing has to be shown. For the other cases we will use induction on the length of a word u . For $\diamond \in \{*, \infty\}$ measurability of $x \mapsto \text{tr}(x)(\{\varepsilon\})$ follows from measurability of $x \mapsto \alpha(x)(\mathbb{1})$ and for $\diamond \in \{\omega, \infty\}$ the function $x \mapsto \text{tr}(x)(\varepsilon A^\diamond)$ is the constant function with value 1 and thus is measurable. Suppose now that for an $n \in \mathbb{N}$ we have established that for all $u \in A^n$ the functions $x \mapsto \text{tr}(x)(\{u\})$ and $x \mapsto \text{tr}(x)(uA^\diamond)$ (whenever they are meaningful) are measurable. Then for all $a \in A$ and all $u \in A^n$ we have $\text{tr}(x)(\{au\}) = \int_{x' \in X} \text{tr}(x')(\{u\}) dP_a(x, x')$ and also $\text{tr}(x)(auA^\diamond) = \int_{x' \in X} \text{tr}(x')(uA^\diamond) dP_a(x, x')$ and by applying Lemma 4.1.17 we get the desired measurability. □

Without any more complicated tools we get the complete result for any \ast -PTS:

Theorem 4.2.20 For all $S \in \mathcal{P}(A^*)$ the function $x \mapsto \text{tr}(x)(S)$ is measurable.

Proof. We know from Lemma 4.2.19 that $x \mapsto \text{tr}(x)(S)$ is measurable for every $S \in \mathcal{S}_\ast$. Recall that $\sigma_{A^*}(\mathcal{S}_\ast) = \mathcal{P}(A^*)$ and every $S \in \mathcal{P}(A^*)$ is at most countably⁷ infinite, say $S := \{u_1, u_2, \dots\}$ and we have the trivial, disjoint decomposition $S = \bigcup_{n=1}^\infty \{u_n\}$. If we define $T_N := \bigcup_{n=1}^N \{u_n\}$ we get an increasing sequence of sets converging to S . Hence by continuity of the subprobability measures $S' \mapsto \text{tr}(x)(S')$ we get $\text{tr}(x)(S) = \lim_{N \rightarrow \infty} \text{tr}(x)(T_N) = \lim_{N \rightarrow \infty} \sum_{n=1}^N \text{tr}(x, \{u_n\})$. Thus $x \mapsto \text{tr}(x)(S)$ is the pointwise limit of a finite sum of measurable functions and therefore measurable. \square

From here until the rest of this subsection we restrict \diamond to be either ω or ∞ if not indicated otherwise. As before, we will rely on transfinite induction for our proof.

Lemma 4.2.21 For every $S \in \mathcal{R}_\diamond(0)$ the function $x \mapsto \text{tr}(x)(S)$ is measurable.

Proof. We know from Lemma 4.2.19 that $x \mapsto \text{tr}(x)(S)$ is measurable for every $S \in \mathcal{S}_\diamond$. Let $S \in \mathcal{R}_\diamond(0)$ then $S = \bigcup_{n=1}^N S_n$ with $S_n \in \mathcal{S}_\diamond$ disjoint for $1 \leq n \leq N \in \mathbb{N}$. We have $\text{tr}(x)(S) = \sum_{n=1}^N \text{tr}(x, S_n)$ which is measurable as a finite sum of measurable functions. \square

Lemma 4.2.22 Let α be an ordinal s.t. the function $x \mapsto \text{tr}(x)(S)$ is measurable for each $S \in \mathcal{R}_\diamond(\alpha)$. Then $x \mapsto \text{tr}(x)(S)$ is measurable for each $S \in \mathcal{J}(\mathcal{R}_\diamond(\alpha))$.

Proof. Let $S \in \mathcal{J}(\mathcal{R}_\diamond(\alpha))$ then $S = \bigcap_{n=1}^\infty S_n$ with $S_n \in \mathcal{R}_\diamond(\alpha)$. We define $T_N := \bigcap_{n=1}^N S_n$ for all $N \in \mathbb{N}$, then $T_N \in \mathcal{R}_\diamond(\alpha)$ by Lemma 4.2.8. We have $T_N \supseteq T_{N+1}$ for all $N \in \mathbb{N}$ and $S = \bigcap_{N=1}^\infty T_N$. Continuity of $S' \mapsto \text{tr}(x)(S')$ for every $x \in X$ yields $\text{tr}(x)(S) = \lim_{N \rightarrow \infty} \text{tr}(x)(T_N)$. Hence $x \mapsto \text{tr}(x)(S)$ is measurable as pointwise limit of measurable functions. \square

Lemma 4.2.23 Let α be an ordinal such that the function $x \mapsto \text{tr}(x)(S)$ is measurable for each $S \in \mathcal{J}(\mathcal{R}_\diamond(\alpha))$. Then $x \mapsto \text{tr}(x)(S)$ is measurable for each $S \in \mathcal{R}_\diamond(\alpha + 1)$.

Proof. Let $S \in \mathcal{R}_\diamond(\alpha + 1)$ then $S = \bigcup_{n=1}^\infty S_n$ with $S_n \in \mathcal{J}(\mathcal{R}_\diamond(\alpha))$. We define $T_N := \bigcup_{n=1}^N S_n$ for all $N \in \mathbb{N}$. Then we know that $T_N \in \mathcal{J}(\mathcal{R}_\diamond(\alpha))$ by Lemma 4.2.9. We have $T_N \subseteq T_{N+1}$ for all $N \in \mathbb{N}$ and $S = \bigcup_{N=1}^\infty T_N$. Continu-

⁷For finite S the proof works analogously but simpler!

ity of the subprobability measures $S' \mapsto \text{tr}(x)(S')$ yields for every $x \in X$ that $\text{tr}(x)(S) = \lim_{N \rightarrow \infty} \text{tr}(x)(T_N)$. Hence the function $x \mapsto \text{tr}(x)(S)$ is measurable as pointwise limit of measurable functions. \square

Lemma 4.2.24 Let γ be a limit ordinal such that for all ordinals $\alpha < \gamma$ the function $x \mapsto \text{tr}(x)(S)$ is measurable for each $S \in \mathcal{R}_\diamond(\alpha)$. Then $x \mapsto \text{tr}(x)(S)$ is measurable for each $S \in \mathcal{R}_\diamond(\gamma)$.

Proof. Let $S \in \mathcal{R}_\diamond(\gamma)$, then there is an $\alpha < \gamma$ such that $S \in \mathcal{R}_\diamond(\alpha)$ and hence $x \mapsto \text{tr}(x)(S)$ is measurable for this S . \square

By using the characterization $\sigma_{A^\diamond}(\mathcal{S}_\diamond) = \mathcal{R}_\diamond(\omega_1)$ of Theorem 4.2.10 and combining the four preceding lemmas we get the desired result:

Theorem 4.2.25 For all $S \in \sigma_{A^\diamond}(\mathcal{S}_\diamond)$ the function $x \mapsto \text{tr}(x)(S)$ is measurable.

Finally, combining this result with Theorem 4.2.12 and the fact that Markov kernels are in one-to-one correspondence with Kleisli arrows [Dob07a, Proposition 2.7] yields:

Theorem 4.2.26 Let $\diamond \in \{0, *, \omega, \infty\}$ and (T, η, μ) be the (sub)probability monad. Then the function $\text{tr}: X \rightarrow TA^\diamond$ given by Definition 4.2.11 is a Kleisli arrow.

4.2.5 The Trace Measure and Final Coalgebra

Before stating the next theorem which presents a close connection between the unique existence of the map into the final coalgebra and the unique extension of a family of σ -finite pre-measures, we first give some intuition: in order to show that a coalgebra is final it is enough to show that every other coalgebra admits a unique homomorphism into it. Commutativity of the square underlying the homomorphism and uniqueness have to be shown for every element of a σ -algebra and one of our main contributions is to reduce the proof obligations to a smaller set of generators, which form a covering semiring. This theorem will later be applied to our four types of transition systems by using the semirings defined earlier and showing that there can be only one way to assign probabilities to their elements.

Theorem 4.2.27 Let (T, η, μ) be either the subprobability monad (S, η, μ) or the probability monad (\mathbb{P}, η, μ) , F be an endofunctor on Meas with a Kleisli law $\lambda: FT \Rightarrow TF$ and (Ω, κ) be an \bar{F} -coalgebra where $\Sigma_{F\Omega} = \sigma_{F\Omega}(\mathcal{S}_{F\Omega})$ for a covering semiring $\mathcal{S}_{F\Omega}$. Then the following statements are equivalent:

1. (Ω, κ) is a final \bar{F} -coalgebra in $\mathcal{Kl}(T)$.
2. For every \bar{F} -coalgebra (X, α) in $\mathcal{Kl}(T)$ there is a unique Kleisli arrow $\text{tr}: X \rightarrow T\Omega$ satisfying the following condition:

$$\forall x \in X, \forall S \in \mathcal{S}_{F\Omega} : \int_{\Omega} p_S \circ \kappa \, d\text{tr}(x) = \int_{FX} p_S \circ \lambda_{\Omega} \circ F(\text{tr}) \, d\alpha(x). \quad (4.2.9)$$

Proof. We consider the final coalgebra diagram in $\mathcal{Kl}(T)$.

$$\begin{array}{ccc} X & \xrightarrow{\alpha} & \bar{F}X \\ \text{tr} \downarrow & & \downarrow \bar{F}(\text{tr}) = \lambda_{\Omega} \circ F(\text{tr}) \\ \Omega & \xrightarrow{\kappa} & \bar{F}\Omega \end{array}$$

By definition (Ω, κ) is final if and only if for every \bar{F} -coalgebra (X, α) there is a unique Kleisli arrow $\text{tr}: X \rightarrow T\Omega$ making the diagram commute. We define

$$g := \mu_{F\Omega} \circ T(\kappa) \circ \text{tr} \text{ (down, right)} \quad \text{and} \quad h := \mu_{F\Omega} \circ T(\bar{F}(\text{tr})) \circ \alpha \text{ (right, down)}$$

and note that commutativity of the final coalgebra diagram is equivalent to

$$\forall x \in X, \forall S \in \mathcal{S}_{F\Omega} : g(x)(S) = h(x)(S) \quad (4.2.10)$$

because $\mathcal{S}_{F\Omega}$ is a covering semiring and for all $x \in X$ both $g(x)$ and $h(x)$ are subprobability measures and thus finite measures which allows us to apply Corollary 4.1.5. We calculate

$$\begin{aligned} g(x)(S) &= (\mu_{F\Omega} \circ T(\kappa) \circ \text{tr})(x)(S) = \mu_{F\Omega}(T(\kappa)(\text{tr}(x)))(S) \\ &= \mu_{F\Omega}(\text{tr}(x) \circ \kappa^{-1})(S) = \int p_S \, d(\text{tr}(x) \circ \kappa^{-1}) = \int p_S \circ \kappa \, d\text{tr}(x) \end{aligned}$$

and if we define $\rho := \bar{F}(\text{tr}) = \lambda_{\Omega} \circ F(\text{tr}): FX \rightarrow TF\Omega$ we obtain

$$\begin{aligned} h(x)(S) &= (\mu_{F\Omega} \circ T(\rho) \circ \alpha)(x)(S) = \mu_{F\Omega}(T(\rho)(\alpha(x)))(S) = \mu_{F\Omega}(\alpha(x) \circ \rho^{-1})(S) \\ &= \int p_S \, d(\alpha(x) \circ \rho^{-1}) = \int p_S \circ \rho \, d\alpha(x) = \int p_S \circ \lambda_{\Omega} \circ F(\text{tr}) \, d\alpha(x) \end{aligned}$$

and thus (4.2.10) is equivalent to (4.2.9). \square

We immediately obtain the following corollary.

Corollary 4.2.28 Let in Theorem 4.2.27 $\kappa = \eta_{F\Omega} \circ \varphi$, for an isomorphism $\varphi: \Omega \rightarrow F\Omega$ in Meas , and let $\mathcal{S}_\Omega \subseteq \mathcal{P}(\Omega)$ be a covering semiring such that $\Sigma_\Omega = \sigma_\Omega(\mathcal{S}_\Omega)$. Then equation (4.2.9) is equivalent to

$$\forall x \in X, \forall S \in \mathcal{S}_\Omega : \quad \text{tr}(x)(S) = \int p_{\varphi(S)} \circ \lambda_\Omega \circ F(\text{tr}) \, d\alpha(x). \quad (4.2.11)$$

Proof. Since φ is an isomorphism in Meas we know from Theorem 4.1.11 that $\Sigma_{F\Omega} = \sigma_{F\Omega}(\varphi(\mathcal{S}_\Omega))$. For every $S \in \mathcal{S}_\Omega$ and every $u \in \Omega$ we calculate

$$p_{\varphi(S)} \circ \kappa(u) = p_{\varphi(S)} \circ \eta_{F\Omega} \circ \varphi(u) = \delta_{\varphi(u)}^{F\Omega}(\varphi(S)) = \chi_{\varphi(S)}(\varphi(u)) = \chi_S(u)$$

and hence we have $\int p_{\varphi(S)} \circ \kappa \, d\text{tr}(x) = \int \chi_S \, d\text{tr}(x) = \text{tr}(x)(S)$. \square

Since we want to apply this corollary to sets of words, we now define the necessary isomorphism φ using the characterization given in Theorem 4.1.11.

Theorem 4.2.29 Let A be an arbitrary alphabet and let

$$\varphi: A^\infty \rightarrow A \times A^\infty + \mathbb{1}, \quad \varepsilon \mapsto \checkmark, \quad au \mapsto (a, u). \quad (4.2.12)$$

Then $\varphi, \varphi|_{A^*}: A^* \rightarrow \varphi(A^*)$ and $\varphi|_{A^\omega}: A^\omega \rightarrow \varphi(A^\omega)$ are isomorphisms in Meas because they are bijective functions⁸ and we have

$$\sigma_{A \times A^\omega}(\varphi(\mathcal{S}_\omega)) = \mathcal{P}(A) \otimes \sigma_{A^\omega}(\mathcal{S}_\omega), \quad (4.2.13)$$

$$\sigma_{A \times A^* + \mathbb{1}}(\varphi(\mathcal{S}_*)) = \mathcal{P}(A) \otimes \sigma_{A^*}(\mathcal{S}_*) \oplus \mathcal{P}(\mathbb{1}), \quad (4.2.14)$$

$$\sigma_{A \times A^\infty + \mathbb{1}}(\varphi(\mathcal{S}_\infty)) = \mathcal{P}(A) \otimes \sigma_{A^\infty}(\mathcal{S}_\infty) \oplus \mathcal{P}(\mathbb{1}). \quad (4.2.15)$$

Proof. Bijectivity is obvious. We will now show validity of (4.2.15), the other equations can be verified analogously.⁹ Let $\mathcal{S}_A := \{\emptyset\} \cup \{\{a\} \mid a \in A\} \cup \{A\}$, then it is easy to show that we have $\sigma_A(\mathcal{S}_A) = \mathcal{P}(A)$ and Theorems 4.1.6 and 4.1.8 yield that

$$\mathcal{P}(A) \otimes \sigma_{A^\infty}(\mathcal{S}_\infty) \oplus \mathcal{P}(\mathbb{1}) = \sigma_{A \times A^\infty + \mathbb{1}}(\mathcal{S}_A * \mathcal{S}_\infty \oplus \mathcal{P}(\mathbb{1})).$$

We calculate $\varphi(\emptyset) = \emptyset$, $\varphi(\{\varepsilon\}) = \mathbb{1}$, $\varphi(\varepsilon A^\omega) = A \times A^\omega$, $\varphi(\varepsilon A^\infty) = A \times A^\infty + \mathbb{1}$, and for all $a \in A$ and all $u \in A^*$ we have $\varphi(\{au\}) = \{(a, u)\}$ and also $\varphi(au A^\infty) = \{a\} \times u A^\infty$. This yields

$$\varphi(\mathcal{S}_\infty) = \{\emptyset, \emptyset + \mathbb{1}, A \times A^\infty + \mathbb{1}\} \cup \{\{a\} \times \{u\} + \emptyset, \{a\} \times u A^\infty + \emptyset \mid a \in A, u \in A^*\}$$

⁸Note that we restrict not only the domain of φ here but also its codomain.

⁹For proving (4.2.14) we can use Theorem 4.1.6 because $\sigma_{A^*}(\mathcal{S}_*) = \sigma_{A^*}(\mathcal{S}_* \cup \{A^*\})$.

and furthermore we have

$$\begin{aligned} \mathcal{S}_A * \mathcal{S}_\infty \oplus \mathcal{P}(\mathbb{1}) = & \{\emptyset, \emptyset + \mathbb{1}\} \cup \{\{\mathbf{a}\} \times \{\mathbf{u}\} + \emptyset, \{\mathbf{a}\} \times \mathbf{u}A^\infty + \emptyset \mid \mathbf{a} \in A, \mathbf{u} \in A^*\} \\ & \cup \{\{\mathbf{a}\} \times \{\mathbf{u}\} + \mathbb{1}, \{\mathbf{a}\} \times \mathbf{u}A^\infty + \mathbb{1} \mid \mathbf{a} \in A, \mathbf{u} \in A^*\} \\ & \cup \{A \times \{\mathbf{u}\} + \emptyset, A \times \mathbf{u}A^\infty + \emptyset \mid \mathbf{u} \in A^*\} \\ & \cup \{A \times \{\mathbf{u}\} + \mathbb{1}, A \times \mathbf{u}A^\infty + \mathbb{1} \mid \mathbf{u} \in A^*\}. \end{aligned}$$

Due to the fact that $A \times A^\infty + \mathbb{1} = A \times \varepsilon A^\infty + \mathbb{1}$ we have $\varphi(\mathcal{S}_\infty) \subseteq \mathcal{S}_A * \mathcal{S}_\infty \oplus \mathcal{P}(\mathbb{1})$ and the monotonicity of the σ -operator yields

$$\sigma_{A \times A^\infty + \mathbb{1}}(\varphi(\mathcal{S}_\infty)) \subseteq \sigma_{A \times A^\infty + \mathbb{1}}(\mathcal{S}_A * \mathcal{S}_\infty \oplus \mathcal{P}(\mathbb{1})).$$

For the other inclusion we remark that

$$\begin{aligned} \{\mathbf{a}\} \times \{\mathbf{u}\} + \mathbb{1} &= (\{\mathbf{a}\} \times \{\mathbf{u}\} + \emptyset) \cup (\emptyset + \mathbb{1}) \\ \{\mathbf{a}\} \times \mathbf{u}A^\infty + \mathbb{1} &= (\{\mathbf{a}\} \times \mathbf{u}A^\infty + \emptyset) \cup (\emptyset + \mathbb{1}) \end{aligned}$$

and together with the countable decomposition $A = \bigcup_{\mathbf{a} \in A} \{\mathbf{a}\}$ it is easy to see that

$$\mathcal{S}_A * \mathcal{S}_\infty \oplus \mathcal{P}(\mathbb{1}) \subseteq \sigma_{A \times A^\infty + \mathbb{1}}(\varphi(\mathcal{S}_\infty))$$

and monotonicity and idempotence of the σ -operator complete the proof. \square

We recall that – in order to get an extension of an endofunctor on Meas – we also need a Kleisli law for the functors and the monads we are using to define PTS. In order to define such a law we first provide two technical lemmas.

Lemma 4.2.30 Let A be an alphabet and (X, Σ_X) be a measurable space.

1. The sets $\mathcal{P}(A) * \Sigma_X$ and $\mathcal{P}(A) * \Sigma_X \oplus \mathcal{P}(\mathbb{1})$ are covering semirings of sets.
2. $\mathcal{P}(A) \otimes \Sigma_X = \sigma_{A \times X}(\mathcal{P}(A) * \Sigma_X)$.
3. $\mathcal{P}(A) \otimes \Sigma_X \oplus \mathcal{P}(\mathbb{1}) = \sigma_{A \times X + \mathbb{1}}(\mathcal{P}(A) * \Sigma_X \oplus \mathbb{1})$.

Proof. Showing property (1) is straightforward and will thus be omitted. The rest follows by Theorems 4.1.6 and 4.1.8. \square

Lemma 4.2.31 (Product Measures) Let A be an alphabet, $\mathbf{a} \in A$ and (X, Σ_X) be a measurable space with a subprobability measure $P: \Sigma_X \rightarrow [0, 1]$. Then the following holds:

1. The *product measure* $\delta_a^A \otimes P: \mathcal{P}(A) \otimes \Sigma_X \rightarrow \mathbb{R}_+$ of δ_a^A and P which is the unique extension of the pre-measure satisfying

$$(\delta_a^A \otimes P)(S_A \times S_X) := \delta_a^A(S_A) \cdot P(S_X) \quad (4.2.16)$$

for all $S_A \times S_X \in \mathcal{P}(A) * \Sigma_X$ is a subprobability measure on $A \times X$. If P is a probability measure on X , then also $\delta_a^A \otimes P$ is a probability measure on $A \times X$.

2. The measure $\delta_a^A \odot P: \mathcal{P}(A) \otimes \Sigma_X \oplus \mathcal{P}(\mathbb{1}) \rightarrow \mathbb{R}_+$ which is defined via the equation

$$(\delta_a^A \odot P)(S) := (\delta_a^A \otimes P)(S \cap (A \times X)) \quad (4.2.17)$$

for all $S \in \mathcal{P}(A) \otimes \Sigma_X \oplus \mathcal{P}(\mathbb{1})$ is a subprobability measure on $A \times X + \mathbb{1}$. If P is a probability measure on X , then also $\delta_a^A \odot P$ is a probability measure on $A \times X + \mathbb{1}$.

Proof. Before proving the statement, we check that the two equations yield unique measures.

1. Existence and uniqueness of the product measure is a well known fact from measure theory and follows immediately by Theorem 4.1.4 because (4.2.16) defines a σ -finite pre-measure on $\mathcal{P}(A) * \Sigma_X$ which by Lemma 4.2.30 is a covering semiring of sets and a generator for the product- σ -algebra.
2. We obviously have non-negativity and $(\delta_a^A \odot P)(\emptyset) = 0$. Let $(S_n)_{n \in \mathbb{N}}$ be a family of pairwise disjoint sets in $\mathcal{P}(A) \otimes \Sigma_X \oplus \mathcal{P}(\mathbb{1})$. Then the following holds

$$\begin{aligned} (\delta_a^A \odot P)\left(\bigcup_{n \in \mathbb{N}} S_n\right) &= (\delta_a^A \otimes P)\left(\bigcup_{n \in \mathbb{N}} (S_n \cap (A \times X))\right) \\ &= \sum_{n \in \mathbb{N}} (\delta_a^A \otimes P)(S_n \cap (A \times X)) = \sum_{n \in \mathbb{N}} (\delta_a^A \odot P)(S_n) \end{aligned}$$

and hence $\delta_a^A \odot P$ as defined by equation (4.2.17) is σ -additive and thus a measure.

For the proof of the Lemma we observe that

$$(\delta_a^A \odot P)(A \times X + \mathbb{1}) = (\delta_a^A \otimes P)(A \times X) = \delta_a^A(A) \cdot P(X) = P(X)$$

which immediately yields that both measures are subprobability measures and if P is a probability measure they are probability measures. \square

With the help of the preceding lemmas, we can now state and prove the Kleisli laws for the endofunctors $A \times _$, $A \times _ + \mathbb{1}$ on Meas and the subprobability monad and the probability monad.

Theorem 4.2.32 (Kleisli Laws for the Probability Monads) Let (T, η, μ) be either the subprobability monad (S, η, μ) or the probability monad (P, η, μ) and A be an alphabet with σ -algebra $\mathcal{P}(A)$.

1. Let $F = A \times _ : \text{Meas} \rightarrow \text{Meas}$. For every measurable space (X, Σ_X) we define

$$\lambda_X : A \times TX \rightarrow T(A \times X), (a, P) \mapsto \delta_a^A \otimes P. \quad (4.2.18)$$

Then $\lambda : FT \Rightarrow TF$ is a Kleisli law.

2. Let $F = A \times _ + \mathbb{1} : \text{Meas} \rightarrow \text{Meas}$. For every measurable space (X, Σ_X) we define

$$\begin{aligned} \lambda_X : A \times TX + \mathbb{1} &\rightarrow T(A \times X + \mathbb{1}) \\ (a, P) &\mapsto \delta_a^A \odot P, \quad \checkmark \mapsto \delta_{\checkmark}^{A \times X + \mathbb{1}}. \end{aligned} \quad (4.2.19)$$

Then $\lambda : FT \Rightarrow TF$ is a Kleisli law.

Proof. In order to show that the given maps are Kleisli laws we have to check commutativity of the following three diagrams

$$\begin{array}{ccccc} \text{FTY} & \xrightarrow{\lambda_Y} & \text{TFY} & & \text{FX} & \xrightarrow{F\eta_X} & \text{FTX} & & \text{FT}^2X & \xrightarrow{\lambda_{TX}} & \text{TFTX} & \xrightarrow{T\lambda_X} & \text{T}^2FX \\ \text{FTf} \downarrow & & \downarrow \text{TFf} & & \searrow \eta_{FX} & & \downarrow \lambda_X & & \downarrow F\mu_X & & & & \downarrow \mu_{FX} \\ \text{FTX} & \xrightarrow{\lambda_X} & \text{TFX} & & & & \text{TFX} & & \text{FTX} & \xrightarrow{\lambda_X} & \text{TFX} & & \text{TFX} \end{array}$$

for all measurable spaces (X, Σ_X) , (Y, Σ_Y) and all measurable functions $f : Y \rightarrow X$. By Lemma 4.2.30 we know that $\mathcal{P}(A) * \Sigma_X$ and $\mathcal{P}(A) * \Sigma_X \oplus \mathcal{P}(\mathbb{1})$ are covering semirings of sets and that they are generators for the σ -algebras $\mathcal{P}(A) \otimes \Sigma_X$ and $\mathcal{P}(A) \otimes \Sigma_X \oplus \mathcal{P}(\mathbb{1})$. Moreover, we know from Lemma 4.2.31 that the measures assigned in equations (4.2.18) and (4.2.19) are subprobability measures and thus finite. We can therefore use Corollary 4.1.5 to check the equality of the various (sub)probability measures. We will provide the proofs for the second Kleisli law only, the proofs for the first law are simpler and can in fact be derived from the given proofs. Let $S := S_A \times S_X + S_{\mathbb{1}} \in \mathcal{P}(A) * \Sigma_X \oplus \mathcal{P}(\mathbb{1})$.

1. Let $f: Y \rightarrow X$ be a measurable function. For $(a, P) \in A \times TY$ we calculate

$$\begin{aligned} (TFf \circ \lambda_Y)(a, P)(S) &= (\delta_a^A \odot P) \left((Ff)^{-1}[S] \right) = (\delta_a^A \odot P)(S_A \times f^{-1}[S_X] + S_{\perp}) \\ &= \delta_a^A(S_A) \cdot P \left(f^{-1}[S_X] \right) = (\delta_a^A \odot (P \circ f^{-1}))(S_A \times S_X + S_{\perp}) \\ &= (\lambda_X \circ FTf)(a, P)(S) \end{aligned}$$

and analogously we obtain

$$\begin{aligned} (TFf \circ \lambda_Y)(\checkmark)(S) &= \delta_{\checkmark}^{A \times Y + \perp} \left((Ff)^{-1}[S] \right) \\ &= \delta_{\checkmark}^{A \times Y + \perp} \left(S_A \times f^{-1}[S_X] + S_{\perp} \right) = \delta_{\checkmark}^{A \times X + \perp}(S) = (\lambda_X \circ FTf)(\checkmark)(S). \end{aligned}$$

2. For $(a, x) \in A \times X$ we calculate

$$\begin{aligned} \eta_{FX}(a, x)(S) &= \delta_{(a, x)}^{FX}(S_A \times S_X + S_{\perp}) = \delta_a^A(S_A) \cdot \delta_x^X(S_X) \\ &= (\delta_a^A \odot \delta_x^X)(S) = \lambda_X(a, \delta_x^X)(S) = (\lambda_X \circ F\eta_X)(a, x)(S) \end{aligned}$$

and also

$$\eta_{FX}(\checkmark) = \delta_{\checkmark}^{FX} = \lambda_X(\checkmark) = \lambda_X(F\eta_X(\checkmark)) = (\lambda_X \circ F\eta_X)(\checkmark).$$

3. For $(a, P) \in FT^2X$ we calculate

$$\begin{aligned} (\lambda_X \circ F\mu_X)(a, P)(S) &= (\lambda_X(a, \mu_X(P)))(S) = (\delta_a^A \odot \mu_X(P))(S) \\ &= \delta_a^A(S_A) \cdot \mu_X(P)(S_X) = \delta_a^A(S_A) \cdot \int p_{S_X} dP \end{aligned}$$

and

$$\begin{aligned} (\mu_{FX} \circ T\lambda_X \circ \lambda_{TX})(a, P)(S) &= \mu_{FX} \left((\delta_a^A \odot P) \circ \lambda_X^{-1} \right)(S) \\ &= \int_{TFX} p_S d \left((\delta_a^A \odot P) \circ \lambda_X^{-1} \right) = \int_{\lambda_X^{-1}(TFX)} p_S \circ \lambda_X d(\delta_a^A \odot P) \\ &= \int_{\{a\} \times TX} p_S \circ \lambda_X d(\delta_a^A \odot P) = \int_{P' \in TX} (\delta_a^A \otimes P')(S) dP(P') \\ &= \int_{P' \in TX} \delta_a^A(S_A) \cdot P'(S_X) dP(P') = \delta_a^A(S_A) \cdot \int p_{S_X} dP. \end{aligned}$$

Analogously we obtain

$$(\lambda_X \circ F\mu_X)(\checkmark) = \lambda_X(\checkmark) = \delta_{\checkmark}^{A \times X + \perp}$$

and

$$\begin{aligned}
 (\mu_{FX} \circ T\lambda_X \circ \lambda_{TX})(\checkmark)(S) &= \mu_{FX} \left(\delta_{\checkmark}^{A \times TX + \mathbb{1}} \circ \lambda_X^{-1} \right) (S) \\
 &= \int_{TFX} p_S d \left(\delta_{\checkmark}^{A \times TX + \mathbb{1}} \circ \lambda_X^{-1} \right) = \int_{\lambda_X^{-1}(TFX)} p_S \circ \lambda_X d\delta_{\checkmark}^{A \times TX + \mathbb{1}} \\
 &= (p_S \circ \lambda_X)(\checkmark) = \delta_{\checkmark}^{A \times X + \mathbb{1}}(S)
 \end{aligned}$$

which concludes the proof. \square

With this result at hand we can finally apply Corollary 4.2.28 to the measurable spaces \emptyset , A^* , A^ω , A^∞ , each of which is of course equipped with the σ -algebra generated by the covering semirings \mathcal{S}_0 , \mathcal{S}_* , \mathcal{S}_ω , \mathcal{S}_∞ as defined in Theorem 4.2.5, to obtain the final coalgebra and the induced trace semantics for PTS as presented in the following theorem.

Theorem 4.2.33 (Final Coalgebra and Trace Semantics for PTS) Let (T, η, μ) be either the subprobability monad (S, η, μ) or the probability monad (P, η, μ) and F be either $A \times _$ or $A \times _ + \mathbb{1}$. A PTS (A, X, α) is an \bar{F} -coalgebra (X, α) in $\mathcal{Kl}(T)$ and vice versa. In the following table we present the (carriers of) final \bar{F} -coalgebras (Ω, κ) in $\mathcal{Kl}(T)$ for all suitable choices of T and F (depending on the type of the PTS).

Type \diamond	Monad T	Endofunctor F	Carrier Ω
\emptyset	S	$A \times _$	$(\emptyset, \{\emptyset\})$
$*$	S	$A \times _ + \mathbb{1}$	$(A^*, \sigma_{A^*}(\mathcal{S}_*))$
ω	P	$A \times _$	$(A^\omega, \sigma_{A^\omega}(\mathcal{S}_\omega))$
∞	P	$A \times _ + \mathbb{1}$	$(A^\infty, \sigma_{A^\infty}(\mathcal{S}_\infty))$

For $\diamond \in \{*, \omega, \infty\}$ we have $\kappa = \eta_{F\Omega} \circ \varphi$ where φ is the isomorphism as defined in Theorem 4.2.29 and for $\diamond = \emptyset$ we take $\kappa = \eta_{F\emptyset} \circ \varphi$ with φ being the empty function $\varphi: \emptyset \rightarrow \emptyset$. The unique arrow into the final coalgebra is the map $\text{tr}: X \rightarrow T\Omega$ given by Definition 4.2.11.

Proof. For the whole proof we always assume that the combinations of the type \diamond of the PTS, the monad T , the endofunctor F and the carrier (Ω, Σ_Ω) are chosen as presented in the table given in the corollary. Thus e.g. $\diamond = *$ automatically yields $T = S$, $F = A \times _ + \mathbb{1}$, $\Omega = A^*$, $\Sigma_\Omega = \sigma_{A^*}(\mathcal{S}_*)$ and we automatically work in the Kleisli category $\mathcal{Kl}(S)$ of the subprobability monad. The first statement of the theorem is obvious by construction of the transition function α . For $\diamond \in \{*, \omega, \infty\}$ we remark that the preconditions of Corollary 4.2.28

are fulfilled and aim at applying this corollary, and especially at evaluating equation (4.2.11) for the covering semirings \mathcal{S}_* , \mathcal{S}_ω , \mathcal{S}_∞ . Let us carry out these calculations in various steps to obtain all the equations of Definition 4.2.11. For all $(b, x') \in A \times X$ we calculate

$$(\lambda_\Omega \circ F(\text{tr}))(b, x') = \begin{cases} \delta_b^A \otimes \text{tr}(x'), & \diamond = \omega \\ \delta_b^A \odot \text{tr}(x'), & \diamond \in \{*, \infty\}. \end{cases}$$

Now suppose S is chosen as $S = \{au\}$, $S = auA^\omega$ or $S = auA^\infty$ respectively for an arbitrary $a \in A$ and an arbitrary $u \in A^*$. Then $\varphi(S) = \{a\} \times S'$ with $S' = \{u\}$, $S' = uA^\omega$ or $S' = uA^\infty$ respectively and hence we obtain

$$\begin{aligned} (p_{\varphi(S)} \circ \lambda_\Omega \circ F(\text{tr}))(b, x') &= \delta_b^A \otimes \text{tr}(x')(\{a\} \times S') \\ &= \delta_b^A(\{a\}) \cdot \text{tr}(x')(S') = \chi_{\{a\} \times X}(b, x') \cdot \text{tr}(x')(S'). \end{aligned}$$

Using this, we evaluate equation (4.2.11) of Corollary 4.2.28 for these sets and get

$$\text{tr}(x)(S) = \int_{(b, x') \in \{a\} \times X} \text{tr}(x')(S') d\alpha(x) = \int_{x' \in X} \text{tr}(x')(S') dP_a(x, x')$$

which yields Equations (4.2.3) and (4.2.5) of Definition 4.2.11. For $\diamond \in \{*, \infty\}$ we calculate

$$(\lambda_\Omega \circ F(\text{tr}))(\checkmark) = \delta_{\checkmark}^{A \times \Omega + 1}$$

and conclude that for $z \in A \times X + 1$ we have $(p_{\varphi(\{\varepsilon\})} \circ \lambda_\Omega \circ F(\text{tr}))(z) = 1$ if and only if $z = \checkmark$. Hence evaluating equation (4.2.11) in this case yields

$$\text{tr}(x)(\{\varepsilon\}) = \int p_{\varphi(\{\varepsilon\})} \circ \lambda_\Omega \circ F(\text{tr}) d\alpha(x) = \int \chi_1 d\alpha(x) = \alpha(x)(1)$$

which is equation (4.2.2). For $\diamond \in \{\omega, \infty\}$ we have $\text{tr}(x)(A^\diamond) = 1$ due to the fact that $\text{tr}(x)$ must be a probability measure. This is already equation (4.2.4) because $A^\diamond = \varepsilon A^\diamond$. Moreover $\varphi(\varepsilon A^\diamond) = \varphi(\Omega) = F\Omega$ and since also $\lambda_\Omega \circ F(\text{tr})$ must be a probability measure evaluating (4.2.11) yields the same:

$$\text{tr}(x)(\varepsilon A^\diamond) = \int p_{\varphi(\varepsilon A^\diamond)} \circ \lambda_\Omega \circ F(\text{tr}) d\alpha(x) = \int 1 d\alpha(x) = \alpha(x)(FX) = 1.$$

Finally, for $\diamond = 0$ we remark that the $\mathcal{Kl}(S)$ -object $(\emptyset, \{\emptyset\})$ is the unique final object of $\mathcal{Kl}(S)$: Given any $\mathcal{Kl}(S)$ -object (X, Σ_X) , the unique map into the final object is given as $f: X \rightarrow S(\emptyset) = \{(p: \{\emptyset\} \rightarrow [0, 1], p(\emptyset) = 0)\}$ mapping any $x \in X$

to the unique element of that set. Moreover, $(\emptyset, \{\emptyset\})$ together with $\kappa = \eta_{F\emptyset} \circ \varphi$, where the map $\varphi: \emptyset \rightarrow A \times \emptyset$ is the obvious and unique isomorphism $(\emptyset, \mathcal{P}(\emptyset)) \cong (A \times \emptyset, \mathcal{P}(A) \otimes \mathcal{P}(\emptyset))$, is a \bar{F} -coalgebra and thus final.

In all cases we have obtained exactly the equations from Definition 4.2.11 which by Theorem 4.2.12 yield a unique function $\text{tr}: X \rightarrow \text{TA}^\diamond$. From Theorem 4.2.26 we know that this function is indeed a Kleisli arrow. \square

4.3 Examples

In this section we will define and examine two truly continuous probabilistic systems and calculate their trace measures or parts thereof. However, in order to deal with these systems, we first need to provide some additional measure theoretic results and tools. At first, we will explain the *counting measure* on countable sets and also the *Lebesgue measure* as this is *the* standard measure on the reals. Afterwards we will take a quick look into the theory of measures with *densities*. With these tools at hand we can finally present the examples. All of the presented results should be contained in any standard textbook on measure and integration theory. We use Jürgen Elstrodt's german textbook *Maß- und Integrationstheorie* [Els11] as our primary source for this short summary.

Definition 4.3.1 (Counting Measure) Let X be a countable set. The *counting measure* on the measurable space $(X, \mathcal{P}X)$ is the cardinality map

$$\#: \mathcal{P}X \rightarrow \overline{\mathbb{R}}_+, \quad A \mapsto |A| \quad (4.3.1)$$

assigning to each finite subset of X its number of elements and ∞ to each infinite subset of X . It is uniquely defined as the extension of the σ -finite pre-measure on the set of all singletons (and \emptyset) which is 1 on every singleton and 0 on \emptyset .

4.3.1 Completion and the Lebesgue Measure

The (one-dimensional) *Lebesgue-Borel measure* is the unique measure λ' on the reals equipped with the Borel σ -algebra $\mathfrak{B}(\mathbb{R})$ satisfying $\lambda'((a, b]) = b - a$ for every $a, b \in \mathbb{R}$, $a \leq b$. In order to obtain the *Lebesgue measure*, we will refine both the measure and the set of measurable sets by *completion*. We call a measure space (X, Σ, μ) *complete* if every subset of a μ -null-set (i.e., a measurable set $S \in \Sigma$ such that $\mu(S) = 0$) is measurable (and necessarily also a μ -null-set). For any measure space (X, Σ, μ) there is always a smallest complete measure space $(X, \tilde{\Sigma}, \tilde{\mu})$ such that $\Sigma \subseteq \tilde{\Sigma}$ and $\tilde{\mu}|_\Sigma = \mu$ called the *completion* [Els11, II. §6]. The completion of the Lebesgue-Borel measure yields the *Lebesgue σ -algebra* \mathcal{L}

and the *Lebesgue measure*¹⁰ $\lambda: \mathcal{L} \rightarrow \overline{\mathbb{R}}$. For the Lebesgue measure we will use the following notation for integrals:

$$\int_a^b f \, dx := \int_{[a,b]} f \, d\lambda.$$

4.3.2 Densities

When dealing with measures on arbitrary measurable spaces – especially in the context of probability measures – it is sometimes useful to describe them using so-called *densities*. We will give a short introduction into the theory of densities here which is sufficient for understanding the upcoming examples. Given a measurable space (X, Σ_X) and measures $\mu, \nu: \Sigma_X \rightarrow \overline{\mathbb{R}}_+$ we call a Borel-measurable function $f: X \rightarrow \overline{\mathbb{R}}$ satisfying

$$\nu(S) = \int_S f \, d\mu \tag{4.3.2}$$

for all measurable sets $S \in \Sigma_X$ a μ -density of ν . In that case $\mu(S) = 0$ implies $\nu(S) = 0$ for all measurable sets $S \in \Sigma_X$ and we say that ν is *absolutely continuous* with respect to μ and write $\nu \ll \mu$. Densities are neither unique nor do they always exist. However, if ν has two μ -densities f, g then $f = g$ holds μ -almost everywhere, i.e., there is a μ null set $N \in \Sigma_X$ such that for all $x \in X \setminus N$ we have $f(x) = g(x)$. Moreover, any such μ -density uniquely defines the measure ν . If $\mu = \lambda$, i.e., μ is the Lebesgue-measure, and (4.3.2) holds for a measure ν and a function f , then f is called *Lebesgue density* of ν . For our examples we will make use of the following result [Els11, IV.2.12 Satz].

Theorem 4.3.2 (Integration and Measures with Densities) Let (X, Σ_X) be a measurable space and let $\mu, \nu: \Sigma_X \rightarrow \overline{\mathbb{R}}_+$ be measures such that ν has a μ -density f . If $g: X \rightarrow \overline{\mathbb{R}}_+$ is ν -integrable, then $\int g \, d\nu = \int gf \, d\mu$.

4.3.3 Examples

With all the previous results at hand, we can now present our two continuous examples using densities to describe the transition functions.

Example 4.3.3 We will first give an informal description of this example as a kind of one-player-game which is played in the closed real interval $[0, 1]$.

¹⁰This is the second meaning of the symbol λ in this chapter. Until here, λ was used as symbol for a Kleisli law.

The player, who is in any point $z \in [0, 1]$, can jump up and will afterwards touch down on a new position $x \in [0, 1]$ which is determined probabilistically. After a jump, the player announces, whether he is left “L” or right “R” of his previous position. The total probability of jumping from z to the left is z and the probability of jumping to the right is $1 - z$. In both cases, we have a continuous uniform probability distribution. As we are within the set of reals, the probability of hitting a specific point $x_0 \in [0, 1]$ is always zero. Let us now continue with the precise definition of our example. Let $A := \{L, R\}$. We consider the PTS $(\{L, R\}, [0, 1], \alpha)$ where $[0, 1]$ is equipped with the Lebesgue σ -algebra of the reals, restricted to that interval denoted $\mathcal{L}([0, 1])$. The transition probability function $\alpha: [0, 1] \rightarrow \mathbb{P}([0, 1])$ is given as

$$\alpha(z)(S) = \int_S f_z d(\# \otimes \lambda)$$

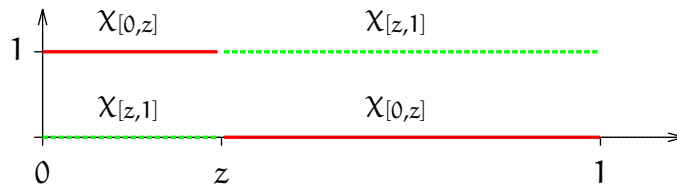
for every $z \in [0, 1]$ and all sets $S \in \mathcal{P}(\{L, R\}) \otimes \mathcal{L}([0, 1])$ with the $(\# \otimes \lambda)$ -densities

$$f_z: \{L, R\} \times [0, 1] \rightarrow \mathbb{R}^+, \quad (a, x) \mapsto \chi_{\{L\} \times [0, z]}(a, x) + \chi_{\{R\} \times [z, 1]}(a, x).$$

We observe that for every real number $z \in [0, 1]$ the functions $S \mapsto P_L(z, S)$, $S \mapsto P_R(z, S): \mathcal{L}([0, 1]) \rightarrow \mathbb{R}^+$ thus have Lebesgue-densities

$$P_L(z, S) = \int_S \chi_{[0, z]} d\lambda = \int_S \chi_{[0, z]}(x) dx, \quad P_R(z, S) = \int_S \chi_{[z, 1]} d\lambda = \int_S \chi_{[z, 1]}(x) dx.$$

with the following graphs (in the real plane)



Evaluating these measures on $[0, 1]$ yields

$$P_L(z, [0, 1]) = \int_0^z 1 dx = z, \quad P_R(z, [0, 1]) = \int_z^1 1 dx = 1 - z.$$

With these preparations at hand we calculate the trace measure on some cones.

$$\begin{aligned}
\text{tr}(z)(\varepsilon A^\omega) &= 1 \\
\text{tr}(z)(L A^\omega) &= \int_{[0,1]} 1 \, dP_L(z, z') = P_L(z, [0, 1]) = z \\
\text{tr}(z)(R A^\omega) &= \int_{[0,1]} 1 \, dP_R(z, z') = P_R(z, [0, 1]) = 1 - z \\
\text{tr}(z)(LL A^\omega) &= \int_{[0,1]} x \, dP_L(z, x) = \int_0^1 x \cdot \chi_{[0,z]}(x) \, dx = \int_0^z x \, dx = \left[\frac{1}{2} x^2 \right]_0^z = \frac{1}{2} z^2 \\
\text{tr}(z)(LR A^\omega) &= \int_{[0,1]} 1 - x \, dP_L(z, x) = \int_0^z (1 - x) \, dx = \left[x - \frac{1}{2} x^2 \right]_0^z = z - \frac{1}{2} z^2 \\
\text{tr}(z)(RL A^\omega) &= \int_{[0,1]} x \, dP_R(z, x) = \int_0^1 x \cdot \chi_{[z,1]}(x) \, dx = \int_z^1 x \, dx = \frac{1}{2} - \frac{1}{2} z^2 \\
\text{tr}(z)(RR A^\omega) &= \int_{[0,1]} 1 - x \, dP_R(z, x) = \int_z^1 (1 - x) \, dx = \frac{1}{2} - z + \frac{1}{2} z^2
\end{aligned}$$

Thus for any word $u \in A^*$ of length n there is a polynomial $p_u \in \mathbb{R}[Z]$ in one variable Z with degree $\deg(p_u) = n$. Evaluating this polynomial for an arbitrary $z \in [0, 1]$ yields the value of the trace measure $\text{tr}(z)$ on the cone uA^ω generated by u , i.e., $\text{tr}(z)(uA^\omega) = p_u(z)$.

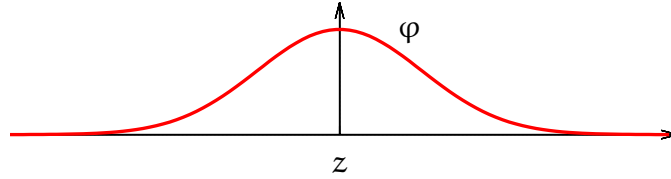
While the previous example provides some understanding on how to describe a continuous PTS and also on how to calculate its trace measure, we are interested in trace equivalence. The second example will thus be a system which is trace equivalent to a finite state system.

Example 4.3.4 As before, we will give an informal description as a kind of one-player-game first. There is exactly one player, who starts in any point $z \in \mathbb{R}$, jumps up and touches down somewhere on the real line announcing whether he is left “L” or right “R” of his previous position or has landed back on his previous position “N”. The probability of landing is initially given via a normal distribution centered on the original position z . Thus, the probability of landing in close proximity of z , i.e., in the interval $[z - \varepsilon, z + \varepsilon]$, is high for sufficiently big $\varepsilon \in \mathbb{R}_+ \setminus \{0\}$ whereas the probability of landing far away, i.e., outside of that interval, is negligible. The player has a finite amount of energy and each jump drains that energy so that after finitely many jumps he will not be able to jump again resulting in an infinite series of “N” messages. Before that the energy level determines the likelihood of his jump width, i.e., the standard deviation of the normal distributions. Now let us give a formal description of such a system.

Recall that the density function of the normal distribution with expected value¹¹ $\mu \in \mathbb{R}$ and standard deviation $\sigma \in \mathbb{R}^+ \setminus \{0\}$ is the Gaussian function

$$\varphi_{\mu,\sigma}: \mathbb{R} \rightarrow \mathbb{R}^+, \quad \varphi_{\mu,\sigma}(x) = \frac{1}{\sigma\sqrt{2\pi}} \cdot \exp\left(-\frac{1}{2} \left(\frac{x-\mu}{\sigma}\right)^2\right)$$

with the following graph (in the real plane), often called the “bell curve”.



Let now the finite “energy level” or “time horizon” (which is the maximal number of jumps) $T \in \mathbb{N}$, $T \geq 2$ be given. We consider the PTS with alphabet $A := \{L, N, R\}$, state space $(\mathbb{N}_0 \times \mathbb{R}, \mathcal{P}(\mathbb{N}_0) \otimes \mathcal{L})$ and transition probability function $\alpha: \mathbb{N}_0 \times \mathbb{R} \rightarrow \mathbb{P}(A \times \mathbb{N}_0 \times \mathbb{R})$ which we define in two steps. For all $(t, z) \in \mathbb{N}_0 \times \mathbb{R}$ with $t < T$ and all measurable sets $S \in \mathcal{P}(A) \otimes \mathcal{P}(\mathbb{N}_0) \otimes \mathcal{L}$ we set

$$\alpha(t, z)(S) := \int_S f_{(t,z)} d(\# \otimes \# \otimes \lambda)$$

where the $(\# \otimes \# \otimes \lambda)$ -density $f_{(t,z)}$ is $f_{(t,z)}: A \times \mathbb{N}_0 \times \mathbb{R} \rightarrow \mathbb{R}^+$, given by

$$f_{(t,z)}(a, t', x) = \begin{cases} \chi_{(-\infty, z]}(x) \cdot \varphi_{z, 1/(t+1)}(x), & a = L \wedge t' = t + 1 \\ \chi_{[z, +\infty)}(x) \cdot \varphi_{z, 1/(t+1)}(x), & a = R \wedge t' = t + 1 \\ 0, & \text{else.} \end{cases}$$

Thus in the first two cases the density is the left (or right) half of the Gaussian density function with expected value $\mu = z$ and standard deviation $\sigma = 1/(t+1)$ and the constant zero function in all other cases. For the remaining $(t, z) \in \mathbb{N}_0 \times \mathbb{R}$ with $t \geq T$ we define the transition probability function to be

$$\alpha(t, z) := \delta_{(N, t+1, z)}^{A \times \mathbb{N}_0 \times \mathbb{R}}.$$

¹¹This is the third meaning of μ . Until here, μ was used as symbol for a measure and also as a symbol for the multiplication natural transformation of a monad.

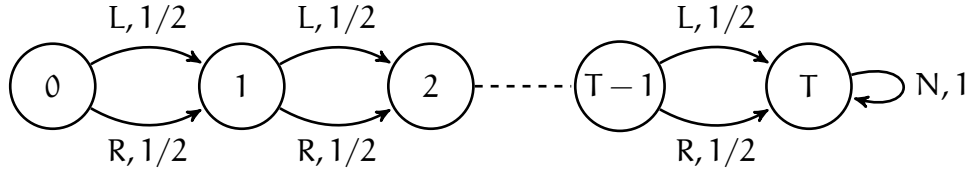
We observe that for $(t, z) \in \mathbb{N}_0 \times \mathbb{R}$ with $t < T$ we have $P_N((t, z), \mathbb{N}_0 \times \mathbb{R}) = 0$ and

$$\begin{aligned} P_L((t, z), \mathbb{N}_0 \times \mathbb{R}) &= \int_{-\infty}^z \varphi_{z, 1/(t+1)}(x) dx = \frac{1}{2} \\ &= \int_z^{\infty} \varphi_{z, 1/(t+1)}(x) dx = P_R((t, z), \mathbb{N}_0 \times \mathbb{R}). \end{aligned}$$

For $t \geq T$ we have $P_N((t, z), \mathbb{N}_0 \times \mathbb{R}) = 1$, $P_L((t, z), \mathbb{N}_0 \times \mathbb{R}) = 0$ and also $P_R((t, z), \mathbb{N}_0 \times \mathbb{R}) = 0$. Once we combine these results we obtain the trace measure. For $t < T$ we get

$$\text{tr}(t, z) = \sum_{u \in \{L, R\}^{T-t}} \left(\frac{1}{2}\right)^{T-t} \cdot \delta_{uN}^{\omega}$$

and for $t \geq T$ the trace measure is $\text{tr}(t, z) = \delta_{N}^{\omega}$. Obviously the trace measure does not depend on z , i.e., $\text{tr}(t, z_1) = \text{tr}(t, z_2)$ for all $t \in \mathbb{N}$ and all $z_1, z_2 \in \mathbb{R}$. Moreover, there is a simple finite state system which is trace equivalent to this system. The finite system has the same alphabet A , its state space is $(\{0, \dots, T\}, \mathcal{P}(\{0, \dots, T\}))$, and the transition function $\alpha: \{0, \dots, T\} \rightarrow \mathbb{P}(A \times \{0, \dots, T\})$ is given as follows



i.e., for $t < T$ we define

$$\alpha(t) = \frac{1}{2} \cdot \left(\delta_{(L, t+1)}^{A \times \{0, \dots, T\}} + \delta_{(R, t+1)}^{A \times \{0, \dots, T\}} \right)$$

and for $t = T$ we define $\alpha(t) = \delta_{(N, T)}^{A \times \{0, \dots, T\}}$.

4.4 Conclusion

We have shown how to obtain coalgebraic trace semantics for generative probabilistic transition systems in a general measure-theoretic setting, thereby allowing not only systems with uncountable state spaces but also the treatment of infinite trace semantics. In particular, we have presented final coalgebras for two functors (with or without termination) on the Kleisli categories of the subprobability and the probability monads yielding a total of four different types of probabilistic systems along with their traces.

4.4.1 Related Work

There is a huge body of work on Markov processes and probabilistic transition systems, but only part of it deals with behavioral equivalences, as in our setting. Even when the focus is on behavioral equivalences, usually bisimilarity and related equivalences are studied (see for instance [LS89; LS91]) instead of the very natural notion of trace equivalence. Furthermore many papers restrict to countable state spaces and discrete probability theory.

Our work is clearly inspired by the Kleisli approach to trace semantics [HJS07], which we generalized to a measure-theoretic setting and considered four slightly different types of systems. Different from the route we took in this chapter – we defined the final coalgebras manually – another option might have been to extend the general theorem of the aforementioned publication [HJS07, Theorem 3.3]. As explained in the Preliminaries (in Section 2.4.3), this theorem gives sufficient conditions under which a final coalgebra in a Kleisli category of a Set-monad arises out of an initial algebra in the underlying category Set. Apart from the fact that the theorem only is stated for Set, it requires that the Kleisli category is cppo-enriched, i.e., that each homset carries a complete partial order with bottom and some additional conditions hold. Thus it is highly non-trivial to generalize. First, it would be necessary to extend it to the category Meas and second – even more importantly – the requirement of the Kleisli category being cppo-enriched is quite restrictive. For the case of the subprobability monad a bottom elements exist (the arrow which maps everything to the constant 0-measure), but this is not the case for the probability monad, which is the more challenging part, giving rise to infinite words. Hence we would require a different theorem, which can also be seen by the fact that in the case of the probability monad the final coalgebra is *not* the initial algebra in Meas.

The study of probabilistic systems using coalgebra is of course not a new approach. Ana Sokolova’s extensive survey on the coalgebraic treatment of discrete systems [Sok11] includes an overview of various different types of transition systems containing probabilistic effects alongside user-input, non-determinism and termination, extensions that we did not consider in this chapter (apart from termination).

The coalgebraic treatment of arbitrary probabilistic systems is the topic of two text books, one by Ernst-Erich Doberkat [Dob07b] and the other one by Prakash Panangaden [Pan09]. Both give a very thorough and general overview of properties of labelled Markov processes including the treatment of probabilistic bisimilarity and its connection to probabilistic temporal logics. Using these logics it is then even possible to define a notion of bisimilarity

distance [Pan09] for such systems. However, both books do not cover the topic of trace equivalences. Moreover, many of the results only can be shown for Polish or analytic spaces instead of general measurable spaces.

Coalgebras for functors on the category *Meas* of measurable spaces and measurable functions have been studied extensively by Ignacio Viglizzo [Vig05b; Vig05a]. In particular, he proves that final coalgebras for measure polynomial functors on *Meas* exist [Vig05a]. However, since all these are coalgebras in *Meas* and not in the Kleisli category over a suitable monad, the obtained behavioral equivalence is probabilistic Larsen-Skou [LS89] bisimilarity instead of trace equivalence and the results do not apply to our setting.

Infinite traces in a general coalgebraic setting have already been studied by Corina Cîrstea [Crs10]. However, this generic theory, once applied to probabilistic systems, is restricted to coalgebras with countable carrier while our setting, which is undoubtedly specific and covers only certain functors and branching types, allows arbitrary carriers for coalgebras of probabilistic systems.

4.4.2 Future Work

As we already pointed out above, we constructed our final coalgebras manually, so one apparent yet likely difficult question is whether there more general approaches to obtain coalgebras in the Kleisli categories of the *Giry* monads.

Another possible future work could be to apply a generic minimization algorithm for coalgebras [ABH+12] and adapt it to this general setting by working out the notion of canonical representatives for probabilistic transition systems. In this case it should be interesting to compare them to the canonical representatives for weak and strong bisimilarity presented recently [EHS+13].

Finally, it might be fruitful to also study probabilistic trace distances coalgebraically as has been done for bisimilarity distances [vBW01b]. This is done for discrete systems in the next chapter but not for the general type of system considered here. Moreover, in this context one could also try to find algorithms for approximating and calculating this distance, perhaps similar to what has been proposed for probabilistic bisimilarity [vBW06; CvBW12] including a recent on-the-fly algorithm [BBLM13].

Behavioral Pseudometrics

IN this final main chapter of the thesis, we aim at taking the coalgebraic behavior analysis one step further by moving from a qualitative analysis to a quantitative one. Thus, instead of considering behavioral *equivalences* coalgebraically, we will develop a coalgebraic framework to obtain canonical definitions for behavioral *pseudometrics*.

Since our approach is heavily influenced by ideas borrowed from transportation theory [Vil09] let us first recall the example from the Introduction (Chapter 1) and discuss how this is related to questions of transportation.

5.1 Motivation

The transition system in Figure 5.1.1 (taken from a paper by Franck van Breugel and James Worrel [vBW06]) is a purely probabilistic transition system with state space $X = \{u, x, y, z\}$ and an arbitrary $\varepsilon \in]0, 1/2[$. An intuitive understanding of such a system is that in each state the system chooses a transition (indicated by the arrows) to another state using the probabilistic information which is given by the numbers on the arrows.

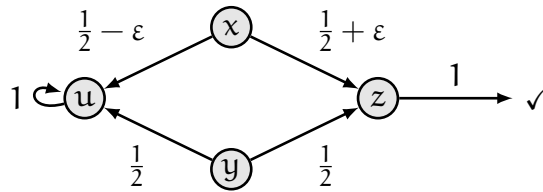


Figure 5.1.1: A probabilistic transition system

The state z on the right hand side of Figure 5.1.1 is a *final state* so the system terminates with probability one (indicated by the arrow to \checkmark) when reaching that state. Contrary to that, state u on the left hand side can be interpreted as a *fail state* which – once reached – can never be left again and the system loops indefinitely in u . Thus the behavior of these states is entirely different.

Comparing the behavior of x and y is a bit more complicated – they both have probabilistic transitions to u and z but in state x there is always a bias towards the final state z which is controlled only by the value of ε . In the Introduction we claimed that due to this x and y are certainly not behaviorally equivalent but similar in the sense that their behavioral distance is ε .

Let us now analyze how we can formally draw that conclusion. First note that we can define a distance between the states u and z based solely on the fact that z is final while u is not. Though we do not yet give it an explicit numerical value, we consider them to be *maximally apart*. Then, in order to compare x and y we need to compare their transitions which (in this example) are probability distributions¹ $P_x, P_y: \{u, z\} \rightarrow [0, 1]$. Thus the underlying task is to *define a distance between probability distributions based on a distance on their common domain of definition*.

Let us now tackle this question with a separate, more illustrative example. We will come back to our probabilistic transition system afterwards (in fact, we will even discuss it more thoroughly throughout the whole chapter).

5.1.1 Wasserstein and Kantorovich Distance

Suppose we are given a three element set $X = \{A, B, C\}$ along with a distance function² $d: X \times X \rightarrow [0, 1]$ where

$$\begin{aligned} d(A, A) &= d(B, B) = d(C, C) = 0, \\ d(A, B) &= d(B, A) = 3, \\ d(A, C) &= d(C, A) = 5, \text{ and} \\ d(B, C) &= d(C, B) = 4. \end{aligned}$$

Based on this function we now want to define a distance on probability distributions on X , i.e., a function $d^{\mathcal{D}}: \mathcal{D}X \times \mathcal{D}X \rightarrow [0, 1]$, so we need to define its value $d^{\mathcal{D}}(P, Q)$ for all probability distributions $P, Q: X \rightarrow [0, 1]$. As a concrete example, let us take the distributions

$$\begin{array}{lll} P(A) = 0.7, & P(B) = 0.1, & P(C) = 0.2, \\ Q(A) = 0.2, & Q(B) = 0.3, \text{ and} & Q(C) = 0.5. \end{array}$$

In order to define their distance, we can interpret the three elements A, B, C as places where a certain product is produced and consumed (imagine the places

¹They are actually probability distributions on X with support $\{u, z\}$. We will discuss this issue later.

²In general we will consider pseudometrics. Here we even have a proper metric.

are coffee roasting plants³, each with an adjacent café where one can taste the coffee). For reasons of simplicity, we assume that the total amount of production equals the amount of consumption⁴. The places are geographically distributed across an area and the distance function just describes their physical distance. Moreover, the above distributions model the supply (P) and demand (Q) of the product in per cent of the total supply or demand. We have illustrated this situation graphically in Figure 5.1.2.

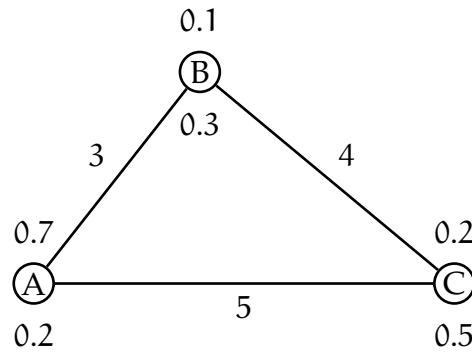


Figure 5.1.2: Lifting example – the numbers on the edges indicate the distance between the places A, B, C whereas the numbers on the nodes indicate supply P (upper value) and demand Q (lower value).

The interpretation given above allows us to find two economically motivated views of defining a distance between P and Q based on the notion of *transportation* which is studied extensively in *transportation theory* [Vil09]. The leading idea is that the product needs to be transported so as to avoid excess supply and meet all demands. As an owner of the three facilities we have two choices: do the transport on our own or find a logistics firm which will do it for us.

If we are organizing the transport ourselves, transporting one unit of our product from one place to another costs one monetary unit per unit of distance travelled. As an example, transporting ten units from A to B will cost $10 \cdot 3 = 30$ monetary units. Formally, we will have to define a function $t: X \times X \rightarrow [0, 1]$ where $t(x, y)$ describes (in %) the amount of goods to be transported from place x to y such that

³Transportation theory was described already in 1781 by the French scientist Gaspard Monge [Mon81]. In his description, an amount of earth which was extracted from the soil (déblais) has to be transported to be used somewhere else (remblais). More recently, mines and factories or bakeries and cafés [Vil09] are used to describe the problem.

⁴If this was not the case we could introduce a dummy place representing either a warehouse (overproduction) or the amount of the product that needs to be bought on the market (underproduction).

- ▷ supplies are used up: for all $x \in X$ we must have $\sum_{y \in X} t(x, y) = P(x)$, and
- ▷ demand is satisfied: for all $y \in X$ we must have $\sum_{x \in X} t(x, y) = Q(y)$.

In probability theory, such a function is as a joint probability distribution with marginals P and Q and is therefore called a *coupling* of P and Q . In our economic perspective we will just call it a *transportation plan* for supply P and demand Q and write $T(P, Q)$ for the set of all such transportation plans.

If $M \in \mathbb{R}_+$ denotes the total supply (= total demand), the total transportation cost for any transportation plan $t \in T(P, Q)$ is given by the linear functional c_d which is parametrized by the distance function d and defined as

$$c_d(t) := \sum_{x, y \in X} (M \cdot t(x, y)) \cdot d(x, y) = M \cdot \sum_{x, y \in X} t(x, y) \cdot d(x, y).$$

Since we want to maximize our profits, we will see to it that the total transportation cost is minimized, i.e., we will look for a transportation plan $t^* \in T(P, Q)$ minimizing the value of c_d (it can be shown that such a t^* always exists). Using this, we can now define the distance of P and Q to be the relative costs $c_d(t^*)/M$ of such an optimal transportation plan, i.e.,

$$d^{\downarrow \mathcal{D}}(P, Q) := \min \left\{ \sum_{x, y \in X} t(x, y) \cdot d(x, y) \mid t \in T(P, Q) \right\}.$$

This distance between probability distributions is called the *Wasserstein distance* and it can be shown that this distance is a pseudometric if d is a pseudometric (and we will recover this result later). In our concrete example of Figure 5.1.2, the best solution is apparently to first use the local production (zero costs) at each facility and then transport the remaining excess supply of 50% in A to the remaining demands in B (20%) and in C (30%). Thus we obtain

$$d^{\downarrow \mathcal{D}}(P, Q) = 0.2 \cdot d(A, B) + 0.3 \cdot d(A, C) = 0.2 \cdot 3 + 0.3 \cdot 5 = 0.6 + 1.5 = 2.1$$

as distance between P and Q yielding an optimal (absolute) transportation cost of $2.1 \cdot M$ monetary units.

If we decide to let a logistics firm do the transportation instead of doing it on our own, we assume that for each place they set up a price for which they will buy a unit of our product (at a place with overproduction) or sell it (at a place with excess demand). Formally it will do so by giving us a price function $f: X \rightarrow \mathbb{R}_+$. We will only accept *competitive price functions* which satisfy

$$|f(x) - f(y)| \leq d(x, y)$$

for all places $x, y \in X$. This amounts to saying that if we sell one unit of our product at place x to the logistics firm and buy one at y it does not cost more than transporting it ourselves from x to y . If d is a pseudometric, we will later call this requirement *non-expansiveness* of the function f . Here, we will denote the set of all these functions by $C(d)$.

The logistics firm is interested in its own profits which are given by the linear functional g_d which is again parametrized by d and defined as

$$g_d(f) := \sum_{x \in X} f(x) \cdot \left((M \cdot Q(x)) - (M \cdot P(x)) \right) = M \cdot \sum_{x \in X} f(x) \cdot (Q(x) - P(x))$$

for all competitive price functions $f \in C(d)$. If in this formula the value $Q(x) - P(x)$ is greater than 0, there is underproduction so the logistics firm can sell goods whereas if $Q(x) - P(x) < 0$ it will have to buy them. Naturally, the logistics firm will want to maximize its profits so it will look for a competitive price function $f^* \in C(d)$ maximizing the value of g_d . Based on this we can now define another distance between P and Q to be the relative profit $g_d(f^*)/M$, i.e.,

$$d^{\uparrow D}(P, Q) := \max \left\{ \sum_{x \in X} f(x) \cdot (Q(x) - P(x)) \mid f \in C(d) \right\}.$$

One can show that for our example it will be best if we give our product to the logistics firm for free⁵ in A , i.e., the logistic firm defines the price $f^*(A) = 0$. Moreover, we need to buy it back at B for three monetary units ($f^*(B) = 3$) and for five monetary units at C ($f^*(C) = 5$). This yields as distance

$$\begin{aligned} d^{\uparrow D}(P, Q) &= \sum_{x \in X} f^*(x) \cdot (Q(x) - P(x)) \\ &= 0 \cdot (0.2 - 0.7) + 3 \cdot (0.3 - 0.1) + 5 \cdot (0.5 - 0.2) = 2.1 \end{aligned}$$

which is exactly the same as the one obtained earlier. In fact, one can prove that $d^{\uparrow D}(P, Q) \leq d^{\downarrow D}(P, Q)$ so whenever we have a transportation plan t^* and a competitive price function f^* so that $c_d(t^*) = g_d(f^*)$ we know that both are optimal yielding $d^{\uparrow D}(P, Q) = d^{\downarrow D}(P, Q) = c_d(t^*)$. As final remark we note that if X is a finite set such a pair (t^*, f^*) will always exist and can be found e.g. using the simplex algorithm from linear programming [Sch99].

5.1.2 Behavioral Distance as Fixed Point

Now that we have finished our little excursion to transportation theory, let us come back to the original example where we wanted to define a distance

⁵Apparently, this is only reasonable in presence of a contract that prohibits the logistics firm to use our product or sell it to anyone else.

between the two states x and y of the probabilistic transition system in Figure 5.1.1. Since we consider u and z to be maximally apart, we could formally set $d(u, z) = d(z, u) = 1$ and $d(u, u) = d(z, z) = 0$ so we obtain as distance function $d: \{u, z\} \times \{u, z\} \rightarrow [0, 1]$ the discrete 1-bounded metric on the set $\{u, z\}$. Using this, we could then define the distance of x and y to be the distance of their transition distributions $P_x, P_y: \{u, z\} \rightarrow [0, 1]$ yielding indeed a distance $d'(x, y) = d^{\downarrow \mathcal{D}}(P_x, P_y) = d^{\uparrow \mathcal{D}}(P_x, P_y) = \varepsilon$ as claimed in the beginning.

However, the remaining question we need to answer is how the above procedure gives rise to a proper behavioral distance in the sense that we obtain a sound and complete definition of a distance function on *the whole set* X , i.e., a pseudometric $d: X \times X \rightarrow [0, 1]$. In order to do that, we just need to observe that the definition of $d'(x, y)$ yields the following fixed point characterization

$$d(x_1, x_2) = d^{\mathcal{D}}(P_{x_1}, P_{x_2}) \quad (5.1.1)$$

for *all* $x_1, x_2 \in X$ where $d^{\mathcal{D}}$ is one of the equivalent distances (Wasserstein or Kantorovich) defined above. A known approach for probabilistic systems as the one above is to define its behavioral distance to be a fixed point $d^*: X \times X \rightarrow [0, 1]$ of the above equation [vBW06; vBSW08]. It is not difficult to see that due to the special structure of the above system, one obtains $d^*(u, z) = d^*(z, u) = 1$ and $d^*(x, y) = d'(x, y) = \varepsilon$ which finally validates our initial claim that the distance of x and y is indeed ε .

5.1.3 Structure of this Chapter

Summing up, we have seen that in order to obtain behavioral distances for probabilistic systems we had to

- ▷ provide a technique to *lift* distances from a set X to the set $\mathcal{D}X$ of probability distributions on it, and
- ▷ solve a fixed point equation involving this lifting on the complete lattice of pseudometrics.

Based on these observations, we will now define a coalgebraic framework to obtain behavioral distances for a large variety of transition systems, not only probabilistic ones. After some preliminary theory on pseudometrics (Section 5.2) and a quick look at some motivating examples (Section 5.3) we will first generalize the Kantorovich/Wasserstein distances: for a given endofunctor F on \mathbf{Set} we define how to obtain a pseudometric d^F on FX based on a given pseudometric d on a set X , which will result in a *lifting* of a \mathbf{Set} endofunctor F to an endofunctor \bar{F} on the category \mathbf{PMet} of pseudometric spaces and nonexpansive functions (Section 5.4).

Then we will prove that we can use a fixed point approach to define a pseudometric on the carrier Z of a final F -coalgebra $z: Z \rightarrow FZ$ which yields the final \bar{F} -coalgebra d_Z (Section 5.5). For any coalgebra $c: X \rightarrow FX$ we can then define the *behavioral distance* of two states x, y to be

$$\text{bd}_c(x, y) := d_Z(\llbracket x \rrbracket_c, \llbracket y \rrbracket_c)$$

thus equipping its carrier X with a canonical pseudometric structure. Moreover, we show that if the lifted functor \bar{F} preserves isometries this pseudometric can directly be computed using a fixed point approach.

As we have discussed extensively in the Preliminaries, the behavioral equivalence induced by the unique homomorphism into the final coalgebra is bisimilarity. Thus it is apparent that our approach described so far yields *bisimilarity pseudometrics*. The remainder of the chapter is therefore devoted to obtaining *trace pseudometrics* via the generalized powerset construction. For this we first study *compositionality* of our lifting approaches (Section 5.6) and then the lifting of *natural transformations* and *monads* (Section 5.7). Using these results, we can then employ the generalized powerset construction to obtain *trace pseudometrics* and show how this applies to nondeterministic and probabilistic automata (Section 5.8). Finally, we will of course discuss related and future work (Section 5.9).

5.2 Pseudometric Spaces

Contrary to the usual definitions, our distances assume values in a closed interval $[0, \top]$, where $\top \in]0, \infty]$ is a fixed maximal element⁶ (for our examples we will use $\top = 1$ or $\top = \infty$). Thus our distances are functions $d: X \times X \rightarrow [0, \top]$. In this way the set of (pseudo)metrics over a fixed set X is a complete lattice (since $[0, \top]$ is) with respect to the pointwise order, i.e., for $d_1, d_2: X \times X \rightarrow [0, \top]$ we define $d_1 \leq d_2$ if and only if $d_1(x, x') \leq d_2(x, x')$ holds for all $x, x' \in X$. We will see later (cf. to Theorem 5.2.8) that the join of a set of pseudometrics is obtained by taking the pointwise supremum of all these functions, whereas the meet cannot be defined in this way (the infimum of a set of pseudometrics need not be a pseudometric). Apart from the completeness, we also ensure that the category whose objects are pseudometric spaces is complete and cocomplete.

Definition 5.2.1 (Pseudometric, Pseudometric Space) Let $\top \in]0, \infty]$ be a fixed maximal distance and X be a set. We call a function $d: X \times X \rightarrow [0, \top]$ a \top -*pseudometric* on X (or a *pseudometric* if \top is clear from the context) if it satisfies

⁶Traditionally distances assume values in $[0, \infty[$.

1. $d(x, x) = 0$ (*reflexivity*),
2. $d(x, y) = d(y, x)$ (*symmetry*), and
3. $d(x, z) \leq d(x, y) + d(y, z)$ (*triangle inequality*)

for all $x, y, z \in X$. If additionally $d(x, y) = 0$ implies $x = y$, d is called a \top -*metric* (or a *metric*). A (pseudo)metric space is a pair (X, d) where X is a set and d is a (pseudo)metric on X .

A trivial example of a pseudometric is the constant 0-function on any set whereas a simple example of a metric is the so-called *discrete metric* which can be defined on any set X as $d(x, x) = 0$ for all $x \in X$ and $d(x, y) = \top$ for all $x, y \in X$ with $x \neq y$.

5.2.1 Calculating with (Extended) Real Numbers

By $d_e: [0, \top]^2 \rightarrow [0, \top]$ we denote the ordinary Euclidean metric on $[0, \top]$, i.e., $d_e(x, y) = |x - y|$ for $x, y \in [0, \top] \setminus \{\infty\}$, and – where appropriate – $d_e(x, \infty) = \infty$ if $x \neq \infty$ and $d_e(\infty, \infty) = 0$. Addition is defined in the usual way, in particular $x + \infty = \infty$ for $x \in [0, \infty]$.

In the following lemma we rephrase the well-known fact that for $a, b, c \in [0, \infty)$ we have $|a - b| \leq c \iff a - b \leq c \wedge b - a \leq c$ to include the cases where a, b, c might be ∞ .

Lemma 5.2.2 For $a, b, c \in [0, \infty]$ we have the following equivalence:

$$d_e(a, b) \leq c \iff (a \leq b + c) \wedge (b \leq a + c).$$

Proof. This equivalence is obvious for $a, b, c \in [0, \infty)$. In the cases $a, b \in [0, \infty]$, $c = \infty$ or $a = b = \infty$, $c \in [0, \infty]$ both sides of the equivalence are true whereas for the cases $a = \infty$, $b, c \in [0, \infty)$ or $b = \infty$, $a, c \in [0, \infty)$ both sides are false. \square

We continue with another simple calculation involving this extended Euclidean distance which will turn out to be useful in the later proofs.

Lemma 5.2.3 For a finite set A and functions $f, g: A \rightarrow [0, \infty]$ we have

1. $d_e(\max_{a \in A} f(a), \max_{a \in A} g(a)) \leq \max_{a \in A} d_e(f(a), g(a))$, and
2. $d_e(\sum_{a \in A} f(a), \sum_{a \in A} g(a)) \leq \sum_{a \in A} d_e(f(a), g(a))$.

Proof. We show both statements separately.

1. Let $a_f \in \arg \max_{a \in A} f(a)$ and $a_g \in \arg \max_{a \in A} g(a)$, i.e., $a_f = \max_{a \in A} f$ and $a_g = \max_{a \in A} g$. If $f(a_f) = g(a_g)$ the left hand side of the above inequality is 0 and so the inequality is satisfied. From here we assume without loss of generality that $f(a_f) > g(a_g)$. Now if $f(a_f) = \infty$, the left hand side is ∞ but also $\max_{a \in A} d_e(f(a), g(a)) \geq d_e(f(a_f), g(a_f)) = \infty$. Finally, for $f(a_f) < \infty$ we have $g(a_f) \leq g(a_g)$ and thus $d_e(f(a_f), g(a_g)) = f(a_f) - g(a_g) \leq f(a_f) - g(a_f) \leq \max_{a \in A} d_e(f(a), g(a))$.
2. Let $s_f := \sum_{a \in A} f(a)$ and $s_g := \sum_{a \in A} g(a)$. If $s_f = s_g$ the left hand side is 0 and the inequality is satisfied. From here we assume without loss of generality $s_f > s_g$. Now if $s_f = \infty$, the left hand side is ∞ but we also must have an $a' \in A$ such that $f(a') = \infty$ (otherwise $s_f < \infty$) and thus $\sum_{a \in A} d_e(f(a), g(a)) \geq d_e(f(a'), g(a')) = \infty$. Finally, for $s_f < \infty$ we have $d_e(s_f, s_g) = s_f - s_g = \sum_{a \in A} f(a) - \sum_{a \in A} g(a) = \sum_{a \in A} (f(a) - g(a)) \leq \sum_{a \in A} |f(a) - g(a)| = \sum_{a \in A} d_e(f(a), g(a))$. \square

Another helpful tool for calculation with the usual (non-extended) reals is the following discrete variant of the Minkowski inequality which arises out of the general version [Ash72, p. 83] by using the counting measure (see Definition 4.3.1) on a finite set.

Theorem 5.2.4 (Minkowski Inequality for Sums) Let $p, n \in \mathbb{N}$ be natural numbers. Then the inequality

$$\left(\sum_{k=1}^n |a_k + b_k|^p \right)^{\frac{1}{p}} \leq \left(\sum_{k=1}^n |a_k|^p \right)^{\frac{1}{p}} + \left(\sum_{k=1}^n |b_k|^p \right)^{\frac{1}{p}}$$

holds for all real numbers $a_k, b_k \in \mathbb{R}$ ($1 \leq k \leq n$).

5.2.2 Pseudometrics Categorically

Having established these few intermediary results, we recall that we want to work in a category whose objects are pseudometric spaces. In order to do so we need to define the arrows between them. While there are other, topologically motivated possibilities (e.g. taking the *continuous* or even *absolutely continuous* functions with respect to the pseudometric topology), we require that our functions do not increase distances.

Definition 5.2.5 (Nonexpansive Function, Isometry) Let $\top \in]0, \infty]$ be an extended real number and (X, d_X) and (Y, d_Y) be \top -pseudometric spaces. We call a function $f: X \rightarrow Y$ *nonexpansive* if

$$d_Y \circ (f \times f) \leq d_X. \quad (5.2.1)$$

In this case we write $f: (X, d_X) \rightarrow (Y, d_Y)$. If equality holds in (5.2.1), f is called an *isometry*.

Note that in this definition we have used a category theoretic mind-set and written (5.2.1) in an “element-free” version as it will be easier to use in some of the subsequent results. Of course, this inequality is equivalent to requiring $d_Y(f(x), f(x')) \leq d_X(x, x')$ for all $x, x' \in X$. Simple examples of nonexpansive functions – even isometries – are of course the identity functions on a set.

Apparently, if these functions shall be the arrows of a category, we will have to check that nonexpansiveness is preserved by function composition.

Lemma 5.2.6 (Composition of Nonexpansive Functions) Let $\top \in]0, \infty]$, and (X, d_X) , (Y, d_Y) and (Z, d_Z) be \top -pseudometric spaces. If $f: (X, d_X) \rightarrow (Y, d_Y)$ and $g: (Y, d_Y) \rightarrow (Z, d_Z)$ are nonexpansive, then so is $g \circ f: (X, d_X) \rightarrow (Z, d_Z)$.

Proof. Using nonexpansiveness of g and f we immediately conclude that

$$d_Z \circ ((g \circ f) \times (g \circ f)) = d_Z \circ (g \times g) \circ (f \times f) \leq d_Y \circ (f \times f) \leq d_X$$

which is the desired nonexpansiveness of $g \circ f$. □

With this result at hand we now give our category a name. Please note that the definition below actually defines a whole family of categories, parametrized by the chosen maximal element \top of the codomain of the pseudometric. Despite of this, we will just speak of *the* category of pseudometric spaces and keep in mind that there are (uncountably) many with the same properties.

Definition 5.2.7 (Category of Pseudometric Spaces) Let $\top \in]0, \infty]$ be a fixed maximal element. The category \mathbf{PMet} has as objects all pseudometric spaces whose pseudometrics have codomain $[0, \top]$. The arrows are the nonexpansive functions between these spaces. The identities are the (isometric) identity functions and composition of arrows is function composition.

This category is complete and cocomplete which in particular implies that it has products and coproducts. We will later see that the respective product and coproduct pseudometrics also arise as special instances of our lifting framework (see Lemmas 5.4.56 and 5.4.60).

Theorem 5.2.8 \mathbf{PMet} is bicomplete, i.e., it is complete and cocomplete.

Proof. Let $D: I \rightarrow \mathbf{PMet}$ be a small diagram, and define $(X_i, d_i) := D(i)$ for each object $i \in I$. Obviously $UD: I \rightarrow \mathbf{Set}$ is also a small diagram. We show

completeness and cocompleteness separately.

Completeness: Let $(f_i: X \rightarrow X_i)_{i \in I}$ be the limit cone to UD in Set. We define the function $d := \sup_{i \in I} d_i \circ (f_i \times f_i) : X^2 \rightarrow [0, \top]$ and claim that this is a pseudometric on X . Since all d_i are pseudometrics, we immediately can derive that $d(x, x) = 0$ and $d(x, y) = d(y, x)$ for all $x, y \in X$. Moreover, for all $x, y, z \in X$:

$$\begin{aligned} d(x, y) + d(y, z) &= \sup_{i \in I} d_i(f_i(x), f_i(y)) + \sup_{i \in I} d_i(f_i(y), f_i(z)) \\ &\geq \sup_{i \in I} (d_i(f_i(x), f_i(y)) + d_i(f_i(y), f_i(z))) \\ &\geq \sup_{i \in I} d_i(f_i(x), f_i(z)) = d(x, z). \end{aligned}$$

With this pseudometric all f_j are nonexpansive functions $(X, d) \rightarrow (X_j, d_j)$. Indeed we have for all $j \in I$ and all $x, y \in X$

$$d_j(f_j(x), f_j(y)) \leq \sup_{i \in I} d_i(f_i(x), f_i(y)) = d(x, y).$$

Moreover, if $(f'_i: (X', d') \rightarrow (X_i, d_i))_{i \in I}$ is a cone to D, $(f'_i: X' \rightarrow X_i)_{i \in I}$ is a cone to UD and hence there is a unique function $g: X' \rightarrow X$ in Set satisfying $f_i \circ g = f'_i$ for all $i \in I$. We finish our proof by showing that this is a nonexpansive function $(X', d') \rightarrow (X, d)$. By nonexpansiveness of the f'_i we have for all $i \in I$ and all $x, y \in X'$ that $d_i(f'_i(x), f'_i(y)) \leq d'(x, y)$ and thus also

$$\begin{aligned} d(g(x), g(y)) &= \sup_{i \in I} d_i(f_i(g(x)), f_i(g(y))) \\ &= \sup_{i \in I} d_i(f'_i(x), f'_i(y)) \leq \sup_{i \in I} d'(x, y) = d'(x, y). \end{aligned}$$

We conclude that $(f_i: (X, d) \rightarrow (X_i, d_i))_{i \in I}$ is a limit cone to D.

Cocompleteness: Let $(f_i: X_i \rightarrow X)_{i \in I}$ be the colimit co-cone from UD in Set and M_X be the set of all pseudometrics $d_X: X^2 \rightarrow [0, \top]$ on X such that the f_i are nonexpansive functions $(X_i, d_i) \rightarrow (X, d_X)$. We define $d := \sup_{d_X \in M_X} d_X$ and claim that this is a pseudometric. Since all d_X are pseudometrics, we can derive immediately that $d(x, x) = 0$ and $d(x, y) = d(y, x)$ for all $x, y \in X$. Moreover, for all $x, y, z \in X$ we have:

$$\begin{aligned} d(x, y) + d(y, z) &= \sup_{d_X \in M_X} d_X(x, y) + \sup_{d_X \in M_X} d_X(y, z) \\ &\geq \sup_{d_X \in M_X} (d_X(x, y) + d_X(y, z)) \geq \sup_{d_X \in M_X} d_X(x, z) = d(x, z). \end{aligned}$$

With this pseudometric all f_j are nonexpansive functions $(X_j, d_j) \rightarrow (X, d)$. Indeed we have for all $j \in I$ and all $x, y \in X_j$

$$d(f_j(x), f_j(y)) = \sup_{d_X \in M_X} d_X(f_j(x), f_j(y)) \leq \sup_{d_X \in M_X} d_j(x, y) = d_j(x, y).$$

Moreover, if $(f'_i: (X_i, d_i) \rightarrow (X', d'))_{i \in I}$ is a co-cone from D , $(f'_i: X_i \rightarrow X')_{i \in I}$ is a co-cone from UD and hence there is a unique function $g: X \rightarrow X'$ in Set satisfying $g \circ f_i = f'_i$ for all $i \in I$. We finish our proof by showing that this is a nonexpansive function $(X, d) \rightarrow (X', d')$. Let $d_g := d' \circ (g \times g): X^2 \rightarrow [0, \top]$, then it is easy to see that d_g is a pseudometric on X . Moreover, for all $i \in I$ and all $x, y \in X_i$ we have

$$d_g(f_i(x), f_i(y)) = d'(g(f_i(x)), g(f_i(y))) = d'(f'_i(x), f'_i(y)) \leq d_i(x, y)$$

due to nonexpansiveness of $f'_i: (X_i, d_i) \rightarrow (X', d')$. Thus all f_i are nonexpansive if seen as functions $(X_i, d_i) \rightarrow (X, d_g)$ and we have $d_g \in M_X$. Using this we observe that for all $x, y \in X$ we have

$$d'(g(x), g(y)) = d_g(x, y) \leq \sup_{d_X \in M_X} d_X(x, y) = d(x, y)$$

which shows that g is a nonexpansive function $(X', d') \rightarrow (X, d)$. We conclude that $(f_i: (X_i, d_i) \rightarrow (X, d))_{i \in I}$ is a colimit co-cone from D . \square

For our purposes it will turn out to be useful to consider the following alternative characterization of the triangle inequality using the concept of nonexpansive functions.

Lemma 5.2.9 A reflexive and symmetric function $d: X^2 \rightarrow [0, \top]$ satisfies the triangle inequality if and only if for all $x \in X$ the function $d(x, _): X \rightarrow [0, \top]$ is a nonexpansive function $d(x, _): (X, d) \rightarrow ([0, \top], d_e)$.

Proof. We show both implications for all $x, y, z \in X$.

- \Rightarrow Using the triangle inequality and symmetry we know that $d(x, y) \leq d(x, z) + d(y, z)$ and $d(x, z) \leq d(x, y) + d(y, z)$. With Lemma 5.2.2 we conclude that $d_e(d(x, y), d(x, z)) \leq d(y, z)$.
- \Leftarrow Using reflexivity of d , the triangle inequality for d_e and nonexpansiveness of $d(x, _)$ we get $d(x, z) = d_e(d(x, x), d(x, z)) \leq d_e(d(x, x), d(x, y)) + d_e(d(x, y), d(x, z)) \leq d(x, y) + d(y, z)$. \square

5.3 Examples of Behavioral Distances

Equipped with this basic knowledge about our pseudometrics, let us now take a look at a few examples which we will use throughout the chapter to demonstrate our theory. All the claims we make in these examples will be justified by our results. Our first example are the purely probabilistic systems like the system in Figure 5.1.1 in the beginning.

Example 5.3.1 (Probabilistic Systems and Behavioral Distance [vBW06]) We consider purely probabilistic transition systems without labels as coalgebras of the form $\alpha: X \rightarrow \mathcal{D}(X + \mathbb{1})$, where \mathcal{D} is the probability distribution functor of Example 2.3.12. Thus $\alpha(x)(y)$, for $x, y \in X$, is the probability of a transition from a state x to y and $\alpha(x)(\checkmark)$ gives the probability of terminating in x .

Franck van Breugel and James Worrell [vBW06] introduced a metric for a continuous version of these systems by considering a discount factor $c \in]0, 1[$. Instantiating their framework to the discrete case we obtain the behavioral distance $d: X^2 \rightarrow [0, 1]$, defined as the least solution (with respect to the order $d_1 \leq d_2 \iff \forall x, y \in X. d_1(x, y) \leq d_2(x, y)$) of the equation

$$d(x, y) = \bar{d}(\alpha(x), \alpha(y))$$

for all $x, y \in X$. The lifted pseudometric $\bar{d}: (\mathcal{D}(X + \mathbb{1}))^2 \rightarrow [0, 1]$ is defined in two steps:

- ▷ First, $\hat{d}: (X + \mathbb{1})^2 \rightarrow [0, 1]$ is defined as $\hat{d}(x, y) = c \cdot d(x, y)$ if $x, y \in X$, $\hat{d}(\checkmark, \checkmark) = 0$ and $\hat{d}(x, y) = 1$ otherwise.
- ▷ Then, for all $P_1, P_2 \in \mathcal{D}(X + \mathbb{1})$, $\bar{d}(P_1, P_2)$ is defined as the supremum of all values $\sum_{x \in X + \mathbb{1}} f(x) \cdot |P_1(x) - P_2(x)|$, with $f: (X + \mathbb{1}, \hat{d}) \rightarrow ([0, 1], d_e)$ being an arbitrary nonexpansive function. This pseudometric is usually called the Kantorovich pseudometric.

Our concrete example from Figure 5.1.1 is an instance of such a system and if we employ the aforementioned approach the behavioral distance of u and z is $d(u, z) = 1$ and hence $d(x, y) = c \cdot \varepsilon$. We will see in Example 5.5.12 that this example can be captured by our framework. Moreover, we will also see that it is possible to set $c = 1$ resulting in $d(x, y) = \varepsilon$.

It is easy to see that also the state space of a deterministic automaton can be equipped with a pseudometric which arises as solution of a fixed point equation.

Example 5.3.2 (Bisimilarity Pseudometric for Deterministic Automata) We consider deterministic automata as coalgebras $\langle o, s \rangle: X \rightarrow 2 \times X^A$ in Set as

discussed after Example 2.4.5. Given a pseudometric $d: X^2 \rightarrow [0, \top]$, we obtain a new pseudometric d^F on $\mathcal{Z} \times X^A$ by defining, for every $(o_1, s_1), (o_2, s_2) \in \mathcal{Z} \times X^A$,

$$d^F((o_1, s_1), (o_2, s_2)) = \max \left\{ d_2(o_1, o_2), c \cdot \max_{a \in A} d(s_1(a), s_2(a)) \right\},$$

where $c \in]0, 1]$ a discount factor and d_2 is the discrete 1-bounded metric on \mathcal{Z} . Using our coalgebra $\langle o, s \rangle: X \rightarrow \mathcal{Z} \times X^A$ we get a fixed point equation on the complete lattice of pseudometrics on X by requiring, for all $x_1, x_2 \in X$,

$$d(x_1, x_2) = \max \left\{ d_2(o(x_1), o(x_2)), c \cdot \max_{a \in A} d(s(x_1)(a), s(x_2)(a)) \right\}.$$

If we take any fixed point of this equation, the distance of two states x_1 and x_2 will be \top if one state is final and the other is not. Otherwise their distance is the c -discounted maximal distance of their successors.

Let us finally consider so-called *metric transition systems* as introduced by Luca de Alfaro, Marco Faella and Mari  lle Stoelinga [dAFSo9]. Each state of such a system comes equipped with a function which maps elements of a set of so-called *propositions* to a kind of non-discrete truth value in a pseudometric space.

Example 5.3.3 (Branching Distance for Metric Transition Systems [dAFSo9])

Let $\Sigma = \{r_1, \dots, r_n\}$ be a finite set of *propositions* where each proposition $r \in \Sigma$ is associated with a pseudometric space (M_r, d_r) which is bounded, i.e., we must have a finite $\top \in]0, \infty[$ such that $d_r: M_r^2 \rightarrow [0, \top]$. A *valuation* of Σ is a function $u: \Sigma \rightarrow \cup_{r \in \Sigma} M_r$ that assigns to each $r \in \Sigma$ an element of M_r , i.e., we require $u(r) \in M_r$. We denote the set of all these valuations by $\mathcal{U}[\Sigma]$ and remark that it is apparently isomorphic to the set $M_1 \times \dots \times M_n$ by means of the bijective function which maps a valuation u to the tuple $(u(r_1), \dots, u(r_n))$.

A *metric transition system* [dAFSo9, Definition 6] is a tuple $(S, \tau, \Sigma, [\cdot])$ with a set S of states, a transition relation $\tau \subseteq S \times S$, a finite set Σ of propositions and a function $[\cdot]: S \rightarrow \mathcal{U}[\Sigma]$ assigning a valuation $[s]$ to each state $s \in S$. We define $\tau(s) := \{s' \in S \mid (s, s') \in \tau\}$ and require that $\tau(s)$ is finite.

The (directed) propositional distance between two valuations $u, v \in \mathcal{U}[\Sigma]$ is given by [dAFSo9, Definition 10]

$$\overline{pd}(u, v) = \max_{r \in \Sigma} d_r(u(r), v(r)).$$

The (undirected) branching distance $d: S \times S \rightarrow \mathbb{R}_0^+$ is defined as [dAFSo9, Definition 13] the smallest fixed-point of the following equation, where $s, t \in S$:

$$d(s, t) = \max \left\{ \overline{pd}([s], [t]), \max_{s' \in \tau(s)} \min_{t' \in \tau(t)} d(s', t'), \max_{t' \in \tau(t)} \min_{s' \in \tau(s)} d(s', t') \right\} \quad (5.3.1)$$

Note that, apart from the first argument, this coincides with the Hausdorff distance between the successors of s and t .

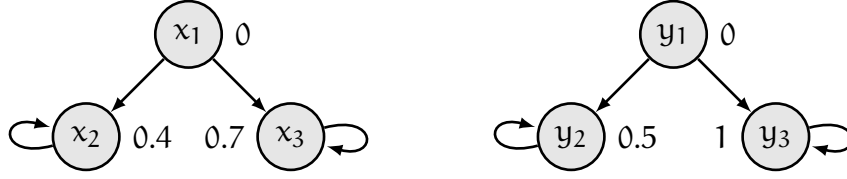


Figure 5.3.1: A metric transition system

We consider the concrete example system in Figure 5.3.1 [dAFS09, Fig. 1] with a single proposition $r \in \Sigma$, where $M_r = [0, 1]$ is equipped with the Euclidean distance d_e . Since the states x_2, x_3, y_2, y_3 only have themselves as successors, computing their distance according to (5.3.1) is easy: we just have to take the propositional distances of the valuations. This results in $d(x_2, y_2) = |0.4 - 0.5| = 0.1$, $d(x_2, y_3) = 0.6$, $d(x_3, y_2) = 0.2$, $d(x_3, y_3) = 0.3$.

Moreover, $\overline{pd}([x_1], [y_1]) = 0$ and thus $d(x_1, y_1)$ equals the Hausdorff distance of the reals associated with the sets of successors which is 0.3 (since this is the maximal distance of any successor to the closest successor in the other set of successors, here: the distance from y_3 to x_3 ; we will provide the details of this computation in Example 5.4.32, page 167).

In order to model such transition systems as coalgebras we consider the product multifunctor $P: \text{Set}^n \rightarrow \text{Set}$ where $P(X_1, \dots, X_n) = X_1 \times \dots \times X_n$. Then coalgebras are of the form $c: S \rightarrow P(M_{r_1}, \dots, M_{r_n}) \times \mathcal{P}_f(S)$, where \mathcal{P}_f is the finite powerset functor and $c(s) = ([s][r_1], \dots, [s][r_n], \tau(s))$. As we will see later in Example 5.5.13, the right-hand side of (5.3.1) can be seen as lifting of a pseudometric d on X to a pseudometric on $P(M_{r_1}, \dots, M_{r_n}) \times \mathcal{P}_f(X)$.

We will later see that in all the examples above, we obtain a coalgebraic *bisimilarity pseudometric*: For any coalgebra $c: X \rightarrow FX$ let us denote the respective least fixed point of Equation (5.1.1) (page 134) by $\text{bd}_c: X^2 \rightarrow [0, \top]$. If a final F-coalgebra $z: Z \rightarrow FZ$ exists and some additional conditions hold (which is the case for our examples) we have

$$\text{bd}_c(x, y) = 0 \quad \Longleftrightarrow \quad \llbracket x \rrbracket_c = \llbracket y \rrbracket_c \quad \Longleftrightarrow \quad x \sim_c y$$

for all $x, y \in X$ where $\llbracket \cdot \rrbracket_c: X \rightarrow Z$ is the map into the final coalgebra and \sim_c is the F-bisimilarity as defined in Definition 2.4.12.

5.4 Lifting Functors to Pseudometric Spaces

Generalizing from our examples, we now establish a general framework for deriving behavioral distances. The crucial step is to find, for an endofunctor F on \mathbf{Set} , a way to transform a pseudometric on X to a pseudometric on FX . This induces a lifting of the functor F in the following sense.

Definition 5.4.1 (Lifting to Pseudometric Spaces) Let $U: \mathbf{PMet} \rightarrow \mathbf{Set}$ be the forgetful functor which maps every pseudometric space to its underlying set. A functor $\bar{F}: \mathbf{PMet} \rightarrow \mathbf{PMet}$ is called a *lifting* of a functor $F: \mathbf{Set} \rightarrow \mathbf{Set}$ if the diagram below commutes.

$$\begin{array}{ccc} \mathbf{PMet} & \xrightarrow{\bar{F}} & \mathbf{PMet} \\ \downarrow U & & \downarrow U \\ \mathbf{Set} & \xrightarrow{F} & \mathbf{Set} \end{array}$$

In this case, for any pseudometric space (X, d) , we denote by d^F the pseudometric on FX which we obtain by applying \bar{F} to (X, d) .

Such a lifting is always monotone on pseudometrics in the following sense.

Theorem 5.4.2 (Monotonicity of Lifting) Let $\bar{F}: \mathbf{PMet} \rightarrow \mathbf{PMet}$ be a lifting of $F: \mathbf{Set} \rightarrow \mathbf{Set}$ and $d_1, d_2: X \times X \rightarrow [0, \top]$ be pseudometrics on X . Then $d_1 \leq d_2$ implies $d_1^F \leq d_2^F$.

Proof. Since $d_1 \leq d_2$ the identity function on the set X can be regarded as a nonexpansive function $f: (X, d_2) \rightarrow (X, d_1)$ because we have for all $x, y \in X$ that $d_1(f(x), f(y)) = d_1(x, y) \leq d_2(x, y)$. By functoriality of \bar{F} we know that also $\bar{F}f: (FX, d_2^F) \rightarrow (FX, d_1^F)$ is nonexpansive, i.e., for all $t_1, t_2 \in FX$ we have $d_1^F(\bar{F}f(t_1), \bar{F}f(t_2)) \leq d_2^F(t_1, t_2)$ and moreover $d_1^F(\bar{F}f(t_1), \bar{F}f(t_2)) = d_1^F(\text{Fid}_X(t_1), \text{Fid}_X(t_2)) = d_1^F(\text{id}_{FX}(t_1), \text{id}_{FX}(t_2)) = d_1^F(t_1, t_2)$ and thus $d_1^F \leq d_2^F$. \square

In order to define a lifting to \mathbf{PMet} we will just use one simple tool, a so-called evaluation function which describes how to transform an element of $F[0, \top]$ to a real number.

Definition 5.4.3 (Evaluation Function & Evaluation Functor) Let F be an endofunctor on \mathbf{Set} . An *evaluation function* for F is a function $\text{ev}_F: F[0, \top] \rightarrow [0, \top]$. Given such a function, we define the *evaluation functor* to be the endofunctor \tilde{F} on

$\text{Set}/[0, \top]$, the slice category⁷ over $[0, \top]$, via $\tilde{F}(g) = \text{ev}_F \circ Fg$ for all $g \in \text{Set}/[0, \top]$. On arrows \tilde{F} is defined as F .

We quickly remark that by definition of \tilde{F} on arrows, it is immediately clear that one indeed obtains a functor so the name is justified.

5.4.1 The Kantorovich Lifting

Let us now consider an endofunctor F on Set with an evaluation function ev_F . Given a pseudometric space (X, d) , our first approach to lift d to FX will be to take the smallest possible pseudometric d^F on FX such that, for all nonexpansive functions $f: (X, d) \rightarrow ([0, \top], d_e)$, also $\tilde{F}f: (FX, d^F) \rightarrow ([0, \top], d_e)$ is nonexpansive again, i.e., we want to ensure that for all $t_1, t_2 \in FX$ we have $d_e(\tilde{F}f(t_1), \tilde{F}f(t_2)) \leq d^F(t_1, t_2)$. This idea immediately leads us to the following definition which corresponds to the maximization of the logistic firm's prices in the introductory example.

Definition 5.4.4 (Kantorovich Function) Let $F: \text{Set} \rightarrow \text{Set}$ be a functor with an evaluation function ev_F . For every pseudometric space (X, d) the *Kantorovich function* on FX is the function $d^{\uparrow F}: FX \times FX \rightarrow [0, \top]$, where

$$d^{\uparrow F}(t_1, t_2) := \sup \left\{ d_e(\tilde{F}f(t_1), \tilde{F}f(t_2)) \mid f: (X, d) \rightarrow ([0, \top], d_e) \right\}$$

for all $t_1, t_2 \in FX$.

Note that a nonexpansive function $f: (X, d) \rightarrow ([0, \top], d_e)$ always exists. If $X = \emptyset$ it is the unique empty function and for $X \neq \emptyset$ every constant function is nonexpansive. Moreover, it is easy to show that $d^{\uparrow F}$ is a pseudometric.

Theorem 5.4.5 (Kantorovich Pseudometric) For every pseudometric space (X, d) the Kantorovich function $d^{\uparrow F}$ is a pseudometric on FX .

Proof. Reflexivity and symmetry are an immediate consequence of the fact that d_e is a metric. We now show the triangle inequality. Let $t_1, t_2, t_3 \in FX$, then

$$\begin{aligned} & d^{\uparrow F}(t_1, t_2) + d^{\uparrow F}(t_2, t_3) \\ &= \sup_{f: (X, d) \rightarrow ([0, \top], d_e)} d_e(\tilde{F}f(t_1), \tilde{F}f(t_2)) + \sup_{f: (X, d) \rightarrow ([0, \top], d_e)} d_e(\tilde{F}f(t_2), \tilde{F}f(t_3)) \end{aligned}$$

⁷The slice category $\text{Set}/[0, \top]$ has as objects all functions $g: X \rightarrow [0, \top]$ where X is an arbitrary set. Given g as before and $h: Y \rightarrow [0, \top]$, an arrow from g to h is a function $f: X \rightarrow Y$ satisfying $h \circ f = g$.

$$\begin{aligned}
 &\geq \sup_{f: (X, d) \rightarrow ([0, \top], d_e)} \left(d_e \left(\tilde{F}f(t_1), \tilde{F}f(t_2) \right) + d_e \left(\tilde{F}f(t_2), \tilde{F}f(t_3) \right) \right) \\
 &\geq \sup_{f: (X, d) \rightarrow ([0, \top], d_e)} d_e \left(\tilde{F}f(t_1), \tilde{F}f(t_3) \right) = d^{\uparrow F}(t_1, t_3)
 \end{aligned}$$

where the first inequality is a simple property of the supremum and the second inequality follows again from the fact that d_e is a metric. \square

Using this pseudometric we can now immediately define our first lifting.

Definition 5.4.6 (Kantorovich Lifting) Let $F: \text{Set} \rightarrow \text{Set}$ be a functor with an evaluation function ev_F . We define the *Kantorovich lifting* of F to be the functor $\bar{F}: \text{PMet} \rightarrow \text{PMet}$, $\bar{F}(X, d) = (FX, d^{\uparrow F})$, $\bar{F}f = Ff$.

Since \bar{F} inherits the preservation of identities and composition of morphisms from F we just need to prove that nonexpansive functions are mapped to nonexpansive functions to obtain functoriality of \bar{F} .

Theorem 5.4.7 The Kantorovich lifting \bar{F} is a functor on pseudometric spaces.

Proof. \bar{F} preserves identities and composition of arrows because F does. Moreover, it preserves nonexpansive functions: Let $f: (X, d_X) \rightarrow (Y, d_Y)$ be nonexpansive and $t_1, t_2 \in FX$, then

$$\begin{aligned}
 d_Y^{\uparrow F}(Ff(t_1), Ff(t_2)) &= \sup_{g: (Y, d_Y) \rightarrow ([0, \top], d_e)} d_e \left(\tilde{F}(g \circ f)(t_1), \tilde{F}(g \circ f)(t_2) \right) \\
 &\leq \sup_{h: (X, d_X) \rightarrow ([0, \top], d_e)} d_e \left(\tilde{F}h(t_1), \tilde{F}h(t_2) \right) = d_X^{\uparrow F}(t_1, t_2)
 \end{aligned}$$

due to the fact that since both f and g are nonexpansive also the composition $(g \circ f): (X, d_X) \rightarrow ([0, \top], d_e)$ is nonexpansive. \square

With this result at hand we are almost done: The only remaining task is to show that \bar{F} is a lifting of F in the sense of Definition 5.4.1 but this is indeed obvious by definition of \bar{F} .

An important property of this lifting is that it preserves isometries, which is a bit tricky to show. While one might be tempted to think that this is immediately true because functors preserve isomorphisms, it is easy to see that the isomorphisms of PMet are the *bijective* isometries. However, there are of course also isometries which are not bijective and thus no isomorphisms. Simple examples for this arise by taking the unique discrete metric space $(\mathbb{1}, d_{\mathbb{1}})$ and mapping it into any other pseudometric space (X, d) with $|X| > 1$. Any function $\mathbb{1} \rightarrow X$ is necessarily isometric but certainly not bijective.

Theorem 5.4.8 The Kantorovich lifting \bar{F} of a functor F preserves isometries.

Proof. Let $f: (X, d_X) \rightarrow (Y, d_Y)$ be an isometry, i.e., f must be a function such that $d_Y \circ (f \times f) = d_X$. Since the Kantorovich lifting \bar{F} is a functor on pseudometric spaces, we already know that $\bar{F}f$ is nonexpansive, i.e., we know that $d_Y^{\uparrow F} \circ (Ff \times Ff) \leq d_X^F$ thus we only have to show the opposite inequality. We will do that by constructing for every nonexpansive function $g: (X, d_X) \rightarrow ([0, \top], d_e)$ a nonexpansive function $h: (Y, d_Y) \rightarrow ([0, \top], d_e)$ such that for every $t_1, t_2 \in FX$ we have equality $d_e(\tilde{F}h(Ff(t_1)), \tilde{F}h(Ff(t_2))) = d_e(\tilde{F}g(t_1), \tilde{F}g(t_2))$, because then we have

$$\begin{aligned} d_Y^{\uparrow F} \circ (Ff \times Ff)(t_1, t_2) &= \sup \left\{ d_e(\tilde{F}h(Ff(t_1)), \tilde{F}h(Ff(t_2))) \mid h: (Y, d_Y) \rightarrow ([0, \top], d_e) \right\} \\ &\geq \sup \left\{ d_e(\tilde{F}g(t_1), \tilde{F}g(t_2)) \mid g: (X, d_X) \rightarrow ([0, \top], d_e) \right\} \\ &= d_X^{\uparrow F}(t_1, t_2). \end{aligned}$$

We construct h as follows: For each $y \in f[X]$ we choose a fixed $x_y \in f^{-1}[\{y\}]$ and define

$$h(y) := \begin{cases} g(x_y), & \text{if } y \in f[X] \\ \inf_{y' \in f[X]} h(y') + d_Y(y', y), & \text{else.} \end{cases}$$

Let us first verify that this definition is independent of our choice of the x_y . Given $x_1, x_2 \in X$ with $f(x_1) = f(x_2) = y$ we get $d_X(x_1, x_2) = d_Y(f(x_1), f(x_2)) = d_Y(y, y) = 0$ using the fact that f is an isometry. Thus by nonexpansiveness of g we necessarily have $d_e(g(x_1), g(x_2)) \leq d_X(x_1, x_2) = 0$ and because d_e is a metric this yields $g(x_1) = g(x_2)$. With the same reasoning we obtain $(h \circ f)(x) = h(f(x)) = g(x_{f(x)}) = g(x)$ for all $x \in X$ and therefore the desired equality

$$d_e(\tilde{F}h(Ff(t_1)), \tilde{F}h(Ff(t_2))) = d_e(\tilde{F}(h \circ f)(t_1), \tilde{F}(h \circ f)(t_2)) = d_e(\tilde{F}g(t_1), \tilde{F}g(t_2)).$$

It remains to show that h is nonexpansive, which we will do by distinguishing three cases.

1. Let $y_1, y_2 \in f[X]$, then there are $x_1, x_2 \in X$ with $f(x_i) = y_i$. We calculate

$$\begin{aligned} d_e(h(y_1), h(y_2)) &= d_e(g(x_1), g(x_2)) \leq d_X(x_1, x_2) \\ &= d_Y(f(x_1), f(x_2)) = d_Y(y_1, y_2) \end{aligned}$$

using nonexpansiveness of g and the fact that f is an isometry.

2. Let without loss of generality⁸ $y_1 \in f[X]$ (so there is $x_1 \in X$ with $f(x_1) = y_1$) and $y_2 \in Y \setminus f[X]$, then by Lemma 5.2.2 we have the equivalence:

$$\begin{aligned} d_e(h(y_1), h(y_2)) &\leq d_Y(y_1, y_2) \\ \iff h(y_1) &\leq h(y_2) + d_Y(y_1, y_2) \quad \wedge \quad h(y_2) \leq h(y_1) + d_Y(y_1, y_2) \end{aligned}$$

We will show these inequalities separately. The second one is easy:

$$h(y_1) + d_Y(y_1, y_2) \geq \inf_{y' \in f[X]} (h(y') + d_Y(y', y_2)) = h(y_2)$$

because $y_1 \in f[X]$. For the first one we calculate

$$\begin{aligned} h(y_2) + d_Y(y_1, y_2) &= \inf_{y' \in f[X]} (h(y') + d_Y(y', y_2)) + d_Y(y_1, y_2) \\ &= \inf_{y' \in f[X]} (h(y') + d_Y(y', y_2) + d_Y(y_2, y_1)) \\ &\geq \inf_{y' \in f[X]} (h(y') + d_Y(y', y_1)) = h(y_1) \end{aligned}$$

using symmetry and the triangle inequality for d_Y . Observe that the last equality is not true by definition because $y_1 \in f[X]$. Certainly we have $h(y_1) = h(y_1) + 0 = h(y_1) + d_Y(y_1, y_1) \geq \inf_{y' \in f[X]} (h(y') + d_Y(y', y_1))$. If we assume this inequality was strict, then there would be $y' \in f[X]$ such that $h(y_1) > h(y') + d_Y(y', y_1)$ which, using Lemma 5.2.2, yields the inequality $d_e(h(y_1), h(y')) > d_Y(y_1, y')$. This contradicts nonexpansiveness of h for elements of $f[X]$. Thus our assumption must have been wrong and the inequality must be an equality.

3. Let $y_1, y_2 \in Y \setminus f[X]$. As in the previous case we use Lemma 5.2.2, however, this time the two inequalities can be shown using exactly the same reasoning. Hence we only show the first one (which in turn is similar as in the prove above):

$$\begin{aligned} h(y_2) + d_Y(y_1, y_2) &= \inf_{y' \in f[X]} (h(y') + d_Y(y', y_2)) + d_Y(y_1, y_2) \\ &= \inf_{y' \in f[X]} (h(y') + d_Y(y', y_2) + d_Y(y_2, y_1)) \\ &\geq \inf_{y' \in f[X]} (h(y') + d_Y(y', y_1)) = h(y_1) \end{aligned}$$

The main difference to the proof above is that the last equality now holds by definition because $y_1 \notin f[X]$. \square

⁸For the case $y_1 \in Y \setminus f[X]$, $y_2 \in f[X]$ we can simply use symmetry of d_e and d_Y .

With this result in place, let us quickly discuss the name of our lifting. We chose the name *Kantorovich* because our definition is reminiscent of the Kantorovich pseudometric in probability theory. If we take the proper combination of functor and evaluation function, we can recover that pseudometric (in the discrete case) as the first instance of our framework.

Example 5.4.9 (Kantorovich Lifting of the Distribution Functor) We take $\top = 1$ and the probability distribution functor \mathcal{D} of Example 2.3.12 (or any of its variants). As evaluation $ev_{\mathcal{D}}: \mathcal{D}[0, 1] \rightarrow [0, 1]$ we define, for each $P \in \mathcal{D}[0, 1]$, $ev(P)$ to be the expected value of the identity function on $[0, 1]$, i.e., $ev_{\mathcal{D}}(P) := \mathbb{E}_P[\text{id}_{[0,1]}] = \sum_{x \in [0,1]} x \cdot P(x)$. Then for any function $g: X \rightarrow [0, 1]$ and any distribution (or subdistribution) $P \in \mathcal{D}X$ we have

$$\begin{aligned} \tilde{\mathcal{D}}g(P) &= ev_{\mathcal{D}} \circ \mathcal{D}g(P) = \mathbb{E}_{\mathcal{D}g(P)}[\text{id}_{[0,1]}] = \sum_{r \in [0,1]} r \cdot \mathcal{D}g(P)(r) \\ &= \sum_{r \in [0,1]} \left(r \cdot \sum_{x \in g^{-1}[\{r\}]} P(x) \right) = \sum_{r \in [0,1]} \sum_{x \in g^{-1}[\{r\}]} r \cdot P(x) \\ &= \sum_{r \in [0,1]} \sum_{x \in g^{-1}[\{r\}]} g(x) \cdot P(x) = \sum_{x \in X} g(x) \cdot P(x). \end{aligned}$$

Using this we calculate, for any nonexpansive function $f: (X, d) \rightarrow ([0, 1], d_e)$ and (sub)probability distributions $P_1, P_2 \in \mathcal{D}X$,

$$\tilde{\mathcal{D}}f(P_1) - \tilde{\mathcal{D}}f(P_2) = \sum_{x \in X} f(x) (P_1(x) - P_2(x)).$$

Thus, for every pseudometric space (X, d) we obtain the Kantorovich pseudometric $d^{\uparrow \mathcal{D}}: (\mathcal{D}X)^2 \rightarrow [0, 1]$, where

$$d^{\uparrow \mathcal{D}}(P_1, P_2) = \sup \left\{ \sum_{x \in X} f(x) \cdot |P_1(x) - P_2(x)| \mid f: (X, d) \rightarrow ([0, 1], d_e) \right\}$$

for all (sub)probability distributions $P_1, P_2: X \rightarrow [0, 1]$.

Let us now consider the question whether the Kantorovich lifting preserves metrics, i.e., we want to check whether the Kantorovich pseudometric $d^{\uparrow \mathcal{F}}$ is a metric for a metric space (X, d) . The next example shows that this is not necessarily the case.

Example 5.4.10 (Kantorovich Lifting of the Squaring Functor) The *squaring functor* on **Set** is the functor $S: \mathbf{Set} \rightarrow \mathbf{Set}$ where $SX = X \times X$ for each set X and $Sf = f \times f$ for each function $f: X \rightarrow Y$ [AHS90, Example 3.20 (10)].

We take $\top = \infty$ as maximal element and consider the evaluation function $ev_S: [0, \infty] \times [0, \infty] \rightarrow [0, \infty]$, $ev_S(r_1, r_2) = r_1 + r_2$.

For a metric space (X, d) with $|X| \geq 2$ take $t_1 = (x_1, x_2) \in SX$ with $x_1 \neq x_2$ and define $t_2 := (x_2, x_1)$. Clearly $t_1 \neq t_2$ but for every nonexpansive function $f: (X, d) \rightarrow ([0, \top], d_e)$ we have $\tilde{S}f(t_1) = f(x_1) + f(x_2) = f(x_2) + f(x_1) = \tilde{S}f(t_2)$ and thus $d^{\uparrow S}(t_1, t_2) = 0$.

5.4.2 The Wasserstein Lifting

We have seen that our first lifting approach bears close resemblance to the original Kantorovich pseudometric on probability measures. We will now also define a generalized version of the Wasserstein pseudometric and compare it with our generalized Kantorovich pseudometric. To do that we first need to define generalized couplings, which can be understood as a generalization of joint probability measures.

Definition 5.4.11 (Coupling) Let $F: \text{Set} \rightarrow \text{Set}$ be a functor and $n \in \mathbb{N}$. Given a set X and $t_i \in FX$ for $1 \leq i \leq n$ we call an element $t \in F(X^n)$ such that $F\pi_i(t) = t_i$ a *coupling* of the t_i (with respect to F). We write $\Gamma_F(t_1, t_2, \dots, t_n)$ for the set of all these couplings.

Using these couplings we now want to proceed to define an alternative pseudometric on FX .

Definition 5.4.12 (Wasserstein Function) Let $F: \text{Set} \rightarrow \text{Set}$ be a functor with evaluation function ev_F . For every pseudometric space (X, d) the *Wasserstein function* on FX is the function $d^{\downarrow F}: FX \times FX \rightarrow [0, \top]$ given by

$$d^{\downarrow F}(t_1, t_2) := \inf \left\{ \tilde{F}d(t) \mid t \in \Gamma_F(t_1, t_2) \right\}. \quad (5.4.1)$$

for all $t_1, t_2 \in FX$.

In contrast to the Kantorovich function, where the respective set cannot be empty because nonexpansive functions always exist, here it might be the case that no coupling exists and thus $d^{\downarrow F}(t_1, t_2) = \inf \emptyset = \top$. Without any additional conditions we cannot even prove that $\Gamma_F(t_1, t_1) \neq \emptyset$ which we would certainly need for reflexivity and thus we do not automatically obtain a pseudometric. The only property we get for free is symmetry.

Lemma 5.4.13 (Symmetry of the Wasserstein Function) For all pseudometric spaces (X, d) the Wasserstein function $d^{\downarrow F}$ is symmetric.

Proof. Let $t_1, t_2 \in FX$ and let $\sigma := \langle \pi_2, \pi_1 \rangle$ be the swap map on $X \times X$, i.e., $\sigma: X \times X \rightarrow X \times X$, $\sigma(x_1, x_2) = (x_2, x_1)$.

If there is a coupling $t_{12} \in \Gamma_F(t_1, t_2)$ we define $t_{21} := F\sigma(t_{12}) \in F(X \times X)$ and observe that it satisfies $F\pi_1(t_{21}) = F\pi_1(F\sigma(t_{12})) = F(\pi_1 \circ \sigma)(t_{12}) = F\pi_2(t_{12}) = t_2$ and analogously $F\pi_2(t_{21}) = t_1$, thus $t_{21} \in \Gamma_F(t_2, t_1)$. Moreover, due to symmetry of d (i.e., $d \circ \sigma = d$), we obtain $\tilde{F}d(t_{21}) = \text{ev}_F(\tilde{F}d(t_{21})) = \text{ev}_F(\tilde{F}d(F\sigma(t_{12}))) = \text{ev}_F(F(d \circ \sigma)(t_{12})) = \text{ev}_F(Fd(t_{12})) = \tilde{F}d(t_{12})$ which yields the desired symmetry.

If no coupling of t_1 and t_2 exists, there is also no coupling of t_2 and t_1 because otherwise we would get a coupling of t_1 and t_2 using the above method. Thus $d^{\downarrow F}(t_1, t_2) = \top = d^{\downarrow F}(t_2, t_1)$ which concludes the proof. \square

In order to be able to guarantee the other two properties of a pseudometric we will restrict our attention to well-behaved evaluation functions.

Definition 5.4.14 (Well-Behaved Evaluation Function) Let ev_F be an evaluation function for a functor $F: \text{Set} \rightarrow \text{Set}$. We call ev_F *well-behaved* if it satisfies the following conditions:

- W1. \tilde{F} is monotone, i.e., for $f, g: X \rightarrow [0, \top]$ with $f \leq g$, we have $\tilde{F}f \leq \tilde{F}g$.
- W2. For any $t \in F([0, \top]^2)$ we have $d_e(\text{ev}_F(t_1), \text{ev}_F(t_2)) \leq \tilde{F}d_e(t)$ for $t_i := F\pi_i(t)$.
- W3. $\text{ev}_F^{-1}[\{0\}] = F i[F\{0\}]$ where $i: \{0\} \hookrightarrow [0, \top]$ is the inclusion map.

While condition W1 is quite natural, for conditions W2 and W3 some explanations are in order. Condition W2 ensures that $\tilde{F}id_{[0, \top]} = \text{ev}_F: F[0, \top] \rightarrow [0, \top]$ is nonexpansive once d_e is lifted to $F[0, \top]$ (recall that for the Kantorovich lifting we require $\tilde{F}f$ to be nonexpansive for *any* nonexpansive f). By definition of the evaluation functor \tilde{F} and the t_i , we have $d_e(\tilde{F}\pi_1(t), \tilde{F}\pi_2(t)) = d_e(\text{ev}_F \circ F\pi_1(t), \text{ev}_F \circ F\pi_2(t)) = d_e(\text{ev}_F(t_1), \text{ev}_F(t_2))$ so Condition W2 can equivalently be stated as $d_e(\tilde{F}\pi_1(t), \tilde{F}\pi_2(t)) \leq \tilde{F}d_e(t)$.

Condition W3 requires that exactly the elements of $F\{0\}$ are mapped to 0 via ev_F . This ensures the reflexivity of the Wasserstein pseudometric.

Lemma 5.4.15 (Reflexivity of the Wasserstein Function) Let F be an endofunctor on Set with evaluation function ev_F . If ev_F satisfies Condition W3 of Definition 5.4.14 then for any pseudometric space (X, d) the Wasserstein function $d^{\downarrow F}$ is reflexive.

Proof. Let $t_1 \in FX$. To show reflexivity we will construct a coupling $t \in \Gamma_F(t_1, t_1)$ such that $\tilde{F}d(t) = 0$. In order to do that, let $\delta: X \rightarrow X^2$, $\delta(x) = (x, x)$ and define $t := F\delta(t_1)$. Then $F\pi_i(t) = F(\pi_i \circ \delta)(t_1) = F(\text{id}_X)(t_1) = t_1$ and thus

$t \in \Gamma_F(t_1, t_1)$. Since d is reflexive, $d \circ \delta: X \rightarrow [0, \top]$ is the constant zero function. Let $i: \{0\} \hookrightarrow [0, \top]$, $i(0) = 0$ and for any set X let $!_X: X \rightarrow \{0\}$, $!_X(x) = 0$. Then also $i \circ !_X: X \rightarrow [0, \top]$ is the constant zero function and thus $d \circ \delta = i \circ !_X$. Using this we can conclude that

$$\tilde{F}d(t) = \tilde{F}d(F\delta(t_1)) = \tilde{F}(d \circ \delta)(t_1) = \tilde{F}(i \circ !_X) = \text{ev}_F\left(Fi((F!_X)(t_1))\right) = 0$$

where the last equality follows from the fact that $F!_X(t_1) \in F\{0\}$ and Condition W_3 of Definition 5.4.14. \square

Before we continue our efforts to obtain a Wasserstein pseudometric, we convince ourselves that well-behaved evaluation functions exist but not every evaluation function is well-behaved.

Example 5.4.16 (Evaluation Function for the Powerset Functor) We take $\top = \infty$ and consider the powerset functor \mathcal{P} of Example 2.3.11. First, we show that the evaluation function $\sup: \mathcal{P}[0, \infty] \rightarrow [0, \infty]$ where $\sup \emptyset := 0$ is well-behaved.

W_1 . Let $f, g: X \rightarrow [0, \infty]$ with $f \leq g$. Let $S \in \mathcal{P}X$, i.e., $S \subseteq X$. Then we have

$$\begin{aligned} \tilde{\mathcal{P}}f(S) &= \sup f[S] = \sup \{f(x) \mid x \in S\} \\ &\leq \sup \{g(x) \mid x \in S\} = \sup g[S] = \tilde{\mathcal{P}}g(S). \end{aligned}$$

W_2 . For any subset $S \subseteq [0, \infty]^2$ we have to show the inequality

$$d_e(\sup \pi_1[S], \sup \pi_2[S]) \leq \sup d_e[S]. \quad (5.4.2)$$

For $S = \emptyset$ this is true because $\sup \emptyset = 0$ and thus both sides of the inequality are 0. Otherwise we define $s_i := \sup \pi_i[S]$. Clearly, if $s_1 = s_2$ then the left hand side of (5.4.2) is 0 and thus the inequality holds. Without loss of generality we now assume $s_1 < s_2$ and distinguish two cases:

1. If $s_2 < \infty$ then for any $\varepsilon > 0$ we can find a pair $(t_1, t_2) \in S$ such that $s_2 - \varepsilon < t_2$ because s_2 is the supremum of $\pi_2[S]$. Moreover, $t_1 \leq s_1$ and if $\varepsilon < s_2 - s_1$ also $t_1 \leq t_2$. By combining these inequalities, we conclude that for every $\varepsilon \in]0, s_2 - s_1[$ we have a pair $(t_1, t_2) \in S$ such that

$$\begin{aligned} d_e(s_1, s_2) - \varepsilon &= s_2 - s_1 - \varepsilon \leq s_2 - t_1 - \varepsilon \\ &= s_2 - \varepsilon - t_1 < t_2 - t_1 = d_e(t_1, t_2). \end{aligned}$$

Since ε can be arbitrarily small, we thus must have (5.4.2).

2. If $s_2 = \infty$ then $d_e(s_1, s_2) = \infty$. However, $s_2 = \infty$ also implies that for every non-negative real number $r \in \mathbb{R}_+$ we can find an element $(t_1, t_2) \in S$ such that $t_2 > r$. Especially, for $r > s_1$ we have $t_2 > r > s_1 \geq t_1$ and thus $d_e(t_1, t_2) = t_2 - t_1 \geq t_2 - s_1 > r - s_1$. Since r can be arbitrarily large, we thus must have $\sup d_e[S] = \infty$ and thus (5.4.2) is an equality.

W_3 . We have $\mathcal{P}i[\mathcal{P}\{0\}] = \mathcal{P}i[\{\emptyset, \{0\}\}] = \{i[\emptyset], i[\{0\}]\} = \{\emptyset, \{0\}\} = \sup^{-1}[\{0\}]$.

Whenever we work with the finite powerset functor \mathcal{P}_f we can of course use \max instead of \sup with the convention $\max \emptyset = 0$.

In contrast to the above, $\inf: \mathcal{P}([0, \infty]) \rightarrow [0, \infty]$ is not well-behaved. It neither satisfies Condition W_2 , nor Condition W_3 : $\inf d_e[S] \geq d_e(\inf \pi_1[S], \inf \pi_2[S])$ fails for $S = \{(0, 1), (1, 1)\}$ and $\{0, 1\} \in \inf^{-1}[\{0\}]$.

Staying with Condition W_3 for a while we remark that it can be expressed as a weak pullback diagram, thus fitting nicely into a coalgebraic framework.

Lemma 5.4.17 (Weak Pullback Characterization of Condition W_3) Let F be an endofunctor on \mathbf{Set} with evaluation function ev_F and $i: \{0\} \hookrightarrow [0, \top]$ be the inclusion function. For any set X we denote the unique arrow into $\{0\}$ by $!_X: X \rightarrow \{0\}$. Then ev_F satisfies Condition W_3 of Definition 5.4.14, i.e., $\text{ev}_F^{-1}[\{0\}] = F[F\{0\}]$ if and only if the diagram below is a weak pullback.

$$\begin{array}{ccc}
 F\{0\} & \xrightarrow{!_{F\{0\}}} & \{0\} \\
 Fi \downarrow & & \downarrow i \\
 F[0, \top] & \xrightarrow{\text{ev}_F} & [0, \top]
 \end{array}$$

Proof. Commutativity of the diagram is equivalent to $\text{ev}_F^{-1}[\{0\}] \supseteq Fi[F\{0\}]$. Given a set X and a function $f: X \rightarrow F[0, \top]$ as depicted below, we conclude again by commutativity ($i \circ !_X = \text{ev}_F \circ f$) that $f(x) \in \text{ev}_F^{-1}[\{0\}]$ for all $x \in X$.

$$\begin{array}{ccccc}
 & & & & \\
 & & & & \\
 X & \xrightarrow{!_X} & F\{0\} & \xrightarrow{!_{F\{0\}}} & \{0\} \\
 & \searrow \varphi & \downarrow Fi & & \downarrow i \\
 & & F[0, \top] & \xrightarrow{\text{ev}_F} & [0, \top] \\
 & \searrow f & & &
 \end{array}$$

Now we show that the weak universality is equivalent to the other inclusion. First suppose that $\text{ev}_F^{-1}[\{0\}] \subseteq \text{Fi}[F\{0\}]$ then for $f(x) \in \text{ev}_F^{-1}[\{0\}]$ we can choose a (not necessarily unique) $x_0 \in F\{0\}$ such that $f(x) = \text{Fi}(x_0)$. If we define $\varphi: X \rightarrow F\{0\}$ by $\varphi(x) = x_0$ then clearly φ makes the above diagram commute and thus we have a weak pullback.

Conversely if the diagram is a weak pullback we consider the set $X = \text{ev}_F^{-1}[\{0\}]$ and the function $f: \text{ev}_F^{-1}[\{0\}] \hookrightarrow F[0, \top]$, $f(x) = x$. Now for any $x \in \text{ev}_F^{-1}[\{0\}]$ we have $\text{Fi}(\varphi(x)) = (\text{Fi} \circ \varphi)(x) = f(x) = x$, hence – since $\varphi(x) \in F\{0\}$ – we have $x \in \text{Fi}[F\{0\}]$. This shows that indeed $\text{ev}_F^{-1}[\{0\}] \subseteq \text{Fi}[F\{0\}]$ holds. \square

The only missing step towards the Wasserstein pseudometric is the observation that if F preserves weak pullbacks we can define new couplings based on given ones.

Lemma 5.4.18 (Gluing Lemma) Let F be an endofunctor on Set , X a set, $t_1, t_2, t_3 \in FX$, $t_{12} \in \Gamma_F(t_1, t_2)$, and $t_{23} \in \Gamma_F(t_2, t_3)$ be couplings. If F preserves weak pullbacks then there is a coupling $t_{123} \in \Gamma_F(t_1, t_2, t_3)$ such that

$$\begin{aligned} F\langle \pi_1, \pi_2 \rangle(t_{123}) &= t_{12} \quad \text{and} \\ F\langle \pi_2, \pi_3 \rangle(t_{123}) &= t_{23} \end{aligned}$$

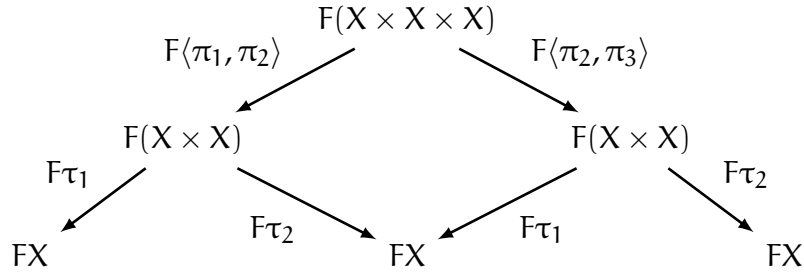
where $\pi_i: X^3 \rightarrow X$ are the projections of the ternary product. Moreover, $t_{13} := F\langle \pi_1, \pi_3 \rangle(t_{123})$ is a coupling of t_1 and t_3 , i.e., we have $t_{13} \in \Gamma_F(t_1, t_3)$.

Proof. Let $\tau_i: X \times X \rightarrow X$ be the projections of the binary product. We first observe that the following diagram is a pullback square.

$$\begin{array}{ccc} & X \times X \times X & \\ \langle \pi_1, \pi_2 \rangle \swarrow & & \searrow \langle \pi_2, \pi_3 \rangle \\ X \times X & & X \times X \\ \tau_2 \searrow & & \swarrow \tau_1 \\ & X & \end{array}$$

Given any set P along with functions $p_1, p_2: P \rightarrow X \times X$ satisfying the condition $\tau_2 \circ p_1 = \tau_1 \circ p_2$ the unique mediating arrow $u: P \rightarrow X \times X \times X$ is given by $u = \langle \tau_1 \circ p_1, \tau_2 \circ p_1, \tau_2 \circ p_2 \rangle = \langle \tau_1 \circ p_1, \tau_1 \circ p_2, \tau_2 \circ p_2 \rangle$.

Now let us look at the following diagram.



Since F preserves weak pullbacks, the square in the middle of this diagram is a weak pullback. We recall that $t_{12} \in \Gamma_F(t_1, t_2)$ and $t_{23} \in \Gamma_F(t_2, t_3)$ so we have $F\tau_2(t_{12}) = t_2 = F\tau_1(t_{23})$. Using this, we can use the (weak) universality of the pullback to obtain⁹ an element $t_{123} \in F(X \times X \times X)$ which satisfies the two equations of the lemma and moreover $F\pi_1(t_{123}) = F(\tau_1 \circ \langle \pi_1, \pi_2 \rangle)(t_{123}) = F\tau_1 \circ F\langle \pi_1, \pi_2 \rangle(t_{123}) = F\tau_1(t_{12}) = t_1$ and analogously $F\pi_2(t_{123}) = t_2$, $F\pi_3(t_{123}) = t_3$ yielding $t_{123} \in \Gamma_F(t_1, t_2, t_3)$.

For $t_{13} := F\langle \pi_1, \pi_3 \rangle(t_{123})$ we calculate $F\tau_1(t_{13}) = F\tau_1(F\langle \pi_1, \pi_3 \rangle(t_{123})) = F(\tau_1 \circ \langle \pi_1, \pi_3 \rangle)(t_{123}) = F\pi_1(t_{123}) = t_1$ and analogously $F\tau_2(t_{13}) = t_3$ so we have $t_{13} \in \Gamma_F(t_1, t_3)$ as claimed. \square

With the help of this lemma we can now finally give sufficient conditions to guarantee that the Wasserstein function satisfies the triangle inequality. Apparently, since we use the above lemma, this will work only for weak pullback preserving functors and we will also need Conditions W1 and W2 of Definition 5.4.14 for the proof.

Lemma 5.4.19 (Triangle Inequality for the Wasserstein Function) Let F be an endofunctor on Set with evaluation function ev_F . If

1. F preserves weak pullbacks and
2. ev_F satisfies Conditions W1 and W2 of Definition 5.4.14

then for any pseudometric space (X, d) the Wasserstein function $d^{\downarrow F}$ satisfies the triangle inequality.

Proof. We will use the characterization of the triangle inequality given by Lemma 5.2.9 (page 140). Hence, given any pseudometric space (X, d) we just have show that for every $t_1 \in FX$ the function $d^{\downarrow F}(t_1, _): (FX, d^{\downarrow F}) \rightarrow ([0, \top], d_e)$

⁹Explicitly: Consider $\{t_2\}$ with functions $p_1, p_2: \{t_2\} \rightarrow F(X \times X)$ where $p_1(t_2) = t_{12}$ and $p_2(t_2) = t_{23}$, then by the weak pullback property there is a (not necessarily unique) function $u: \{t_2\} \rightarrow F(X \times X \times X)$ satisfying $F(\langle \pi_1, \pi_2 \rangle) \circ u = p_1$ and $F(\langle \pi_2, \pi_3 \rangle) \circ u = p_2$. We simply define $t_{123} := u(t_2)$.

is nonexpansive, i.e., that the inequality

$$d_e(d^{\downarrow F}(t_1, t_2), d^{\downarrow F}(t_1, t_3)) \leq d^{\downarrow F}(t_2, t_3) \quad (5.4.3)$$

holds for all $t_2, t_3 \in FX$. We will show this in several steps.

First of all we consider the case where no coupling of t_2 and t_3 exists. In this case the right hand side of (5.4.3) is \top and it is easy to see that the left hand side can never exceed that value because $d^{\downarrow F}$ is non-negative. Thus in the remainder of the proof we only consider the case where $\Gamma_F(t_2, t_3) \neq \emptyset$.

As next step we observe that if $\Gamma_F(t_1, t_2) = \Gamma_F(t_1, t_3) = \emptyset$ the left hand side of (5.4.3) is 0 and the right hand side is non-negative. Thus we are left with the cases where $\Gamma_F(t_1, t_2) \neq \emptyset$ or $\Gamma_F(t_1, t_3) \neq \emptyset$.

Let us first assume that $\Gamma_F(t_1, t_2) \neq \emptyset$ and recall that we required $\Gamma_F(t_2, t_3) \neq \emptyset$. With the Gluing Lemma (Lemma 5.4.18) we can then conclude that also $\Gamma_F(t_1, t_3) \neq \emptyset$. Similarly, if $\Gamma_F(t_1, t_3) \neq \emptyset$ we can use the swap map as in the proof of Lemma 5.4.13 to see that $\Gamma_F(t_3, t_1) \neq \emptyset$. As above the Gluing Lemma yields $\Gamma_F(t_2, t_1) \neq \emptyset$ and again using the swap map we conclude that $\Gamma_F(t_1, t_2) \neq \emptyset$. Thus the sole remaining case is the case where all couplings exists, i.e., we have $\Gamma_F(t_1, t_2) \neq \emptyset$, $\Gamma_F(t_2, t_3) \neq \emptyset$ and $\Gamma_F(t_1, t_3) \neq \emptyset$.

As intermediary step we recall that for all $x \in X$ the function $d(x, _)$ is nonexpansive (see Lemma 5.2.9, page 140). Using the projections $\pi_i: X^3 \rightarrow X$ of the product this can be formulated as the inequality

$$d_e \circ (d \times d) \circ \langle \langle \pi_1, \pi_2 \rangle, \langle \pi_1, \pi_3 \rangle \rangle \leq d \circ \langle \pi_2, \pi_3 \rangle$$

and the monotonicity of \tilde{F} (Condition W1) implies that also the inequality

$$\tilde{F}(d_e \circ (d \times d) \circ \langle \langle \pi_1, \pi_2 \rangle, \langle \pi_1, \pi_3 \rangle \rangle) \leq \tilde{F}(d \circ \langle \pi_2, \pi_3 \rangle) \quad (5.4.4)$$

holds. We will now use this inequality to prove (5.4.3) for the remaining case in which all couplings exists.

As already pointed out before, for any $t_{12} \in \Gamma_F(t_1, t_2)$ and $t_{23} \in \Gamma_F(t_2, t_3)$ the Gluing Lemma (Lemma 5.4.18) yields a $t_{123} \in \Gamma_F(t_1, t_2, t_3)$ and a coupling $t_{13} := F(\langle \pi_1, \pi_3 \rangle)(t_{123}) \in \Gamma_F(t_1, t_3)$. Plugging in t_{123} in the inequality (5.4.4) above yields $\tilde{F}d_e(F(d \times d)(t_{12}, t_{13})) \leq \tilde{F}d(t_{23})$. Using well-behavedness (Condition W2) of ev_F on the left hand side we obtain the following, intermediary result:

$$d_e(\tilde{F}d(t_{12}), \tilde{F}d(t_{13})) \leq \tilde{F}d(t_{23}). \quad (5.4.5)$$

If we define $d_{ij} := d^{\downarrow F}(t_i, t_j)$ we can express (5.4.3) as $d_e(d_{12}, d_{13}) \leq d_{23}$. This is obviously true for $d_{12} = d_{13}$ so without loss of generality we assume $d_{12} < d_{13}$

and claim that for all $\varepsilon > 0$ there is a coupling $t_{12} \in \Gamma_F(t_1, t_2)$ such that for all couplings $t_{13} \in \Gamma_F(t_1, t_3)$ we have

$$d_e(d_{12}, d_{13}) \leq \varepsilon + d_e(\tilde{F}d(t_{12}), \tilde{F}d(t_{13})). \quad (5.4.6)$$

To prove this claim, we recall that the Wasserstein distance is defined as an infimum, so we have $d_{13} \leq \tilde{F}d(t_{13})$ for all couplings t_{13} . Moreover, for the same reason we can pick, for every $\varepsilon > 0$, a coupling $t_{12} \in \Gamma_F(t_1, t_2)$, such that $\tilde{F}d(t_{12}) - d_{12} \leq \varepsilon$ which can equivalently be stated as $\tilde{F}d(t_{12}) \leq d_{12} + \varepsilon$. With this fixed coupling we now proceed to establish (5.4.4) for all $t_{13} \in \Gamma_F(t_1, t_3)$.

If $d_{13} = \infty$ we have $d_e(d_{12}, d_{13}) = \infty$ but also $\tilde{F}d(t_{13}) = \infty$ and $\tilde{F}d(t_{12}) \leq d_{12} + \varepsilon < \infty + \varepsilon = \infty$ and therefore $d_e(\tilde{F}d(t_{12}), \tilde{F}d(t_{13})) = \infty$ and thus (5.4.6) is valid. For $d_{13} < \infty$ we have

$$\begin{aligned} d_e(d_{12}, d_{13}) &= d_{13} - d_{12} \leq \tilde{F}d(t_{13}) - (\tilde{F}d(t_{12}) - \varepsilon) = \varepsilon + (\tilde{F}d(t_{13}) - \tilde{F}d(t_{12})) \\ &\leq \varepsilon + |\tilde{F}d(t_{13}) - \tilde{F}d(t_{12})| \leq \varepsilon + d_e(\tilde{F}d(t_{12}), \tilde{F}d(t_{13})) \end{aligned}$$

where the last inequality is due to the fact that $\tilde{F}d(t_{12}) < \infty$. Hence we have established our claimed validity of (5.4.6). Using this, (5.4.5) and the fact that – as above – given $\varepsilon > 0$ we have a coupling t_{23} such that $\tilde{F}d(t_{23}) \leq d_{23} + \varepsilon$ we obtain the inequality

$$d_e(d_{12}, d_{13}) \leq \varepsilon + d_e(\tilde{F}d(t_{12}), \tilde{F}d(t_{13})) \leq \varepsilon + \tilde{F}d(t_{23}) \leq 2\varepsilon + d_{23}$$

which also proves $d_e(d_{12}, d_{13}) \leq d_{23}$. Indeed if $d_e(d_{12}, d_{13}) > d_{23}$ then we would have $d_e(d_{12}, d_{13}) = d_{23} + \varepsilon'$ and we just take $\varepsilon < \varepsilon'/2$ which yields the contradiction $d_e(d_{12}, d_{13}) \leq 2\varepsilon + d_{23} < \varepsilon' + d_{23} = d_e(d_{12}, d_{13})$. \square

Combining this result with our previous considerations we finally obtain the desired result which guarantees that the Wasserstein function is indeed a pseudometric.

Theorem 5.4.20 (Wasserstein Pseudometric) Let F be an endofunctor on \mathbf{Set} with evaluation function ev_F . If

1. F preserves weak pullbacks and
2. ev_F is well-behaved

then for any pseudometric space (X, d) the Wasserstein function $d^{\downarrow F}$ is a pseudometric.

Proof. Reflexivity is given by Lemma 5.4.15, symmetry by Lemma 5.4.13 and the triangle inequality by Lemma 5.4.19. \square

With this result in place we can now finally study the Wasserstein lifting of a functor. Of course, our requirements on F and ev_F are just sufficient conditions to prove that the Wasserstein function is a pseudometric so it might be possible to give a more general definition. However, we will always work with weak pullback preserving functors and well-behaved evaluation functions so the following definition suffices.

Definition 5.4.21 (Wasserstein Lifting) Let F be a weak pullback preserving endofunctor on Set with well-behaved evaluation function ev_F . We define the *Wasserstein lifting* of F to be the functor $\bar{F}: \text{PMet} \rightarrow \text{PMet}$, $\bar{F}(X, d) = (FX, d^{\downarrow F})$, $\bar{F}f = Ff$.

Of course, we will have to check the functoriality. Its proof relies on Condition W_1 of Definition 5.4.14, the monotonicity of \bar{F} .

Theorem 5.4.22 The Wasserstein lifting \bar{F} is a functor on pseudometric spaces.

Proof. \bar{F} preserves identities and composition of arrows because F does. Moreover, it preserves nonexpansive functions: Let $f: (X, d_X) \rightarrow (Y, d_Y)$ be nonexpansive and $t_1, t_2 \in FX$. Every $t \in \Gamma_F(t_1, t_2)$ satisfies $Ff(t_i) = Ff(F\pi_i(t)) = F(f \circ \pi_i)(t) = F(\pi_i \circ (f \times f))(t) = F\pi_i(F(f \times f)(t))$. Hence we can calculate

$$\begin{aligned} d_X^{\downarrow F}(t_1, t_2) &= \inf \left\{ \tilde{F}d_X(t) \mid t \in \Gamma_F(t_1, t_2) \right\} \\ &\geq \inf \left\{ \tilde{F}d_X(t) \mid t \in F(X \times X), F\pi_i(F(f \times f)(t)) = Ff(t_i) \right\} \end{aligned} \quad (5.4.7)$$

$$\begin{aligned} &\geq \inf \left\{ \tilde{F}d_Y(F(f \times f)(t)) \mid t \in F(X \times X), F\pi_i(F(f \times f)(t)) = Ff(t_i) \right\} \\ &\quad (5.4.8) \end{aligned}$$

$$\geq \inf \left\{ \tilde{F}d_Y(t') \mid t' \in \Gamma_F(Ff(t_1), Ff(t_2)) \right\} = d_Y^{\downarrow F}(Ff(t_1), Ff(t_2)). \quad (5.4.9)$$

In this calculation the inequality (5.4.7) is due to our initial observation. Furthermore, (5.4.8) holds because f is nonexpansive, i.e., $d_X \geq d_Y \circ (f \times f)$ and applying the monotonicity (Condition W_1 of Definition 5.4.14) of \bar{F} yields $\tilde{F}d_X \geq \tilde{F}(d_Y \circ (f \times f)) = \tilde{F}d_Y \circ F(f \times f)$. The last inequality, (5.4.9), is due to the fact that there might be more couplings t' than those obtained via $F(f \times f)$. \square

Let us now study the properties of the Wasserstein lifting. As was the case for the Kantorovich lifting, also the Wasserstein lifting preserves isometries.

Theorem 5.4.23 The Wasserstein lifting \bar{F} of a functor F preserves isometries.

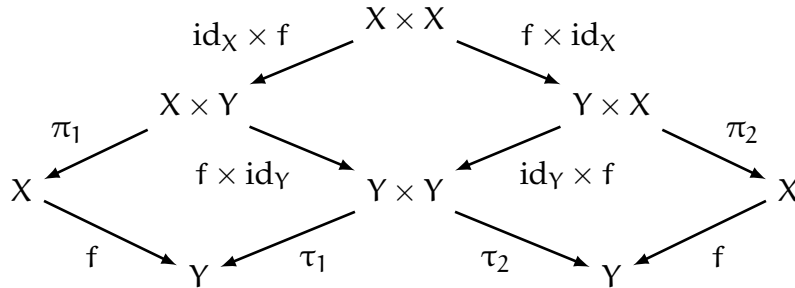
Proof. Let $f: (X, d_X) \rightarrow (Y, d_Y)$ be an isometry. Since \bar{F} is a functor, $\bar{F}f$ is non-expansive, i.e., for all $t_1, t_2 \in FX$ we have $d_X^{\downarrow F}(t_1, t_2) \geq d_Y^{\downarrow F}(Ff(t_1), Ff(t_2))$. Now we show the opposite direction, i.e., that for all $t_1, t_2 \in FX$ we have $d_X^{\downarrow F}(t_1, t_2) \leq d_Y^{\downarrow F}(Ff(t_1), Ff(t_2))$.

If $\Gamma_F(Ff(t_1), Ff(t_2)) = \emptyset$ we have $d_Y^{\downarrow F}((Ff(t_1), Ff(t_2))) = \top \geq d_X^{\downarrow F}(t_1, t_2)$. Otherwise we will construct for each coupling $t \in \Gamma_F(Ff(t_1), Ff(t_2))$ a coupling $\gamma(t) \in \Gamma_F(t_1, t_2)$ such that $\tilde{F}d_X(\gamma(t)) = \tilde{F}d_Y(t)$ because then we have

$$\begin{aligned} d_X^{\downarrow F}(t_1, t_2) &= \inf_{t' \in \Gamma_F(t_1, t_2)} \tilde{F}d_X(t') \leq \inf_{t \in \Gamma_F(Ff(t_1), Ff(t_2))} \tilde{F}d_X(\gamma(t)) \\ &= \inf_{t \in \Gamma_F(Ff(t_1), Ff(t_2))} \tilde{F}d_Y(t) = d_Y^{\downarrow F}(Ff(t_1), Ff(t_2)) \end{aligned}$$

as desired. In this calculation the inequality is due to the fact that $\gamma(t) \in \Gamma_F(t_1, t_2)$ is a coupling and there might be other couplings which are not in the image of γ .

In order to construct $\gamma: \Gamma_F(Ff(t_1), Ff(t_2)) \rightarrow \Gamma_F(t_1, t_2)$, we consider the diagram below where $\pi_1: X \times Y \rightarrow X$, $\pi_2: Y \times X \rightarrow Y$, and $\tau_i: Y \times Y \rightarrow Y$ are the respective projections of the products.

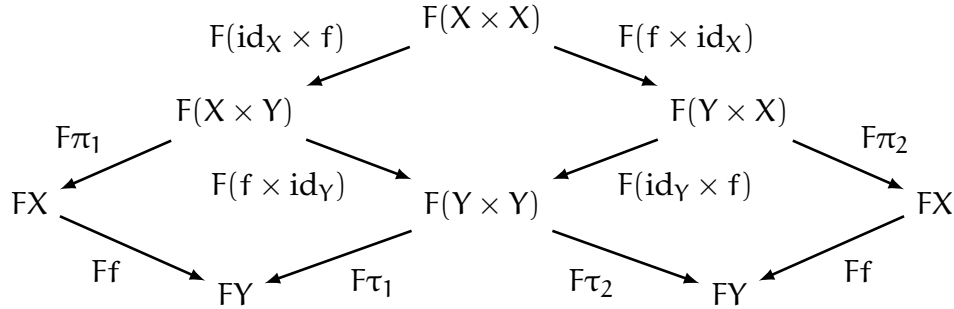


This diagram consists of pullbacks: it is easy to check that the diagram commutes. The unique mediating arrows are constructed as follows.

- ▷ For the lower left part let P be a set with $p_1: P \rightarrow X$, $p_2: P \rightarrow Y \times Y$ such that $f \circ p_1 = \tau_1 \circ p_2$, then define $u: P \rightarrow X \times Y$ as $u := \langle p_1, \tau_2 \circ p_2 \rangle$.
- ▷ Analogously, for the lower right part let P be a set with $p_1: P \rightarrow Y \times Y$, $p_2: P \rightarrow X$ such that $\tau_2 \circ p_1 = f \circ p_2$, then define $u: P \rightarrow X \times Y$ as $u := \langle \tau_1 \circ p_1, p_2 \rangle$.

- ▷ Finally, for the upper part let P be a set with $p_1: P \rightarrow X \times Y$, $p_2: P \rightarrow Y \times X$ such that $(f \times \text{id}_Y) \circ p_1 = (\text{id}_Y \times f) \circ p_2$, then define $u: P \rightarrow X \times X$ as $u := \langle \pi_1 \circ p_1, \pi_2 \circ p_2 \rangle$.

We apply the weak pullback preserving functor F to the diagram and obtain the following diagram which hence consists of three weak pullbacks.



Given a coupling $t \in \Gamma_F(Ff(t_1), Ff(t_2)) \subseteq F(Y \times Y)$ we know $F\tau_i(t) = Ff(t_i) \in FY$.

Since the lower left square in the diagram is a weak pullback, we obtain an element¹⁰ $s_1 \in F(X \times Y)$ with $F\pi_1(s_1) = t_1$ and $F(f \times \text{id}_Y)(s_1) = t$. Similarly, from the lower right square, we obtain $s_2 \in F(Y \times X)$ with $F\pi_2(s_2) = t_2$ and $F(\text{id}_Y \times f)(s_2) = t$. Again by the weak pullback property we obtain our $\gamma(t) \in F(X \times X)$ with $F(\text{id}_X \times f)(\gamma(t)) = s_1$, $F(f \times \text{id}_X)(\gamma(t)) = s_2$.

We convince ourselves that $\gamma(t)$ is indeed a coupling of t_1 and t_2 : Let $\pi'_i: X \times X \rightarrow X$ be the missing projections. Using $\pi_1 \circ (\text{id}_X \times f) = \pi'_1$ we have

$$F\pi'_1(\gamma(t)) = F(\pi_1 \circ (\text{id}_X \times f))(\gamma(t)) = F\pi_1 \circ F(\text{id}_X \times f)(\gamma(t)) = F\pi_1(s_1) = t_1$$

and analogously

$$F\pi'_2(\gamma(t)) = F(\pi_2 \circ (f \times \text{id}_X))(\gamma(t)) = F\pi_2 \circ F(f \times \text{id}_X)(\gamma(t)) = F\pi_2(s_2) = t_2.$$

Moreover, using $f \times f = (f \times \text{id}_Y) \circ (\text{id}_X \times f)$ and functoriality we have

$$\begin{aligned} F(f \times f)(\gamma(t)) &= F((f \times \text{id}_Y) \circ (\text{id}_X \times f))(\gamma(t)) \\ &= F(f \times \text{id}_Y) \circ F(\text{id}_X \times f)(\gamma(t)) = F(f \times \text{id}_Y)(s_1) = t \end{aligned}$$

and thus $\tilde{F}d_Y(t) = \tilde{F}d_Y(F(f \times f)(\gamma(t))) = \tilde{F}(d_Y \circ (f \times f))(t) = \tilde{F}(d_X(t))$ as desired. Note that the last equality is due to the fact that f is an isometry. \square

In contrast to the Kantorovich lifting, we can prove that metrics are preserved by the Wasserstein lifting in certain situations.

¹⁰See the proof of Lemma 5.4.18 for the explicit constructions.

Theorem 5.4.24 (Preservation of Metrics) Let F be a weak pullback preserving endofunctor on \mathbf{Set} with well-behaved evaluation function ev_F and (X, d) be a metric space. If for all $t_1, t_2 \in FX$ where $d^{\downarrow F}(t_1, t_2) = 0$ there is an optimal F -coupling $\gamma(t_1, t_2) \in \Gamma_F(t_1, t_2)$ such that $0 = d^{\downarrow F}(t_1, t_2) = \tilde{F}d(\gamma(t_1, t_2))$ then $d^{\downarrow F}$ is a metric and thus $\bar{F}(X, d) = (FX, d^{\downarrow F})$ is a metric space.

Proof. Let (X, d) be a metric space. We know from Theorem 5.4.20 that $d^{\downarrow F}$ is a pseudometric. Thus we just have to show that for any $t_1, t_2 \in FX$ the fact that $d^{\downarrow F}(t_1, t_2) = 0$ implies $t_1 = t_2$.

Since d is a metric the preimage $d^{-1}[\{0\}]$ is the set $\Delta_X = \{(x, x) \mid x \in X\}$. Hence the square on the left below is a pullback and adding the projections yields $\pi_1 \circ e = \pi_2 \circ e$ where $e: \Delta_X \hookrightarrow X \times X$ is the inclusion. Furthermore, by Lemma 5.4.17 we know that due to Condition W_3 of Definition 5.4.14 the square on the right is a weak pullback.

$$\begin{array}{ccc}
 \Delta_X & \xrightarrow{!_{\Delta_X}} & \{0\} \\
 e \downarrow & & \downarrow i \\
 X \xleftarrow[\pi_2]{\pi_1} X \times X & \xrightarrow{d} & [0, \top]
 \end{array}
 \qquad
 \begin{array}{ccc}
 F\{0\} & \xrightarrow{!_{F\{0\}}} & \{0\} \\
 Fi \downarrow & & \downarrow i \\
 F[0, \top] & \xrightarrow{\text{ev}_F} & [0, \top]
 \end{array}$$

Since F preserves weak pullbacks, applying it to the first diagram yields a weak pullback. By combining this diagram with the right diagram we obtain the diagram below where the outer rectangle is again a weak pullback.

$$\begin{array}{ccccc}
 F\Delta_X & \xrightarrow{F!_{\Delta_X}} & F\{0\} & \xrightarrow{!_{F\{0\}}} & \{0\} \\
 Fe \downarrow & & \downarrow Fi & & \downarrow i \\
 FX \xleftarrow[F\pi_2]{F\pi_1} F(X \times X) & \xrightarrow{Fd} & F[0, \top] & \xrightarrow{\text{ev}_F} & [0, \top] \\
 & & \searrow \tilde{F}d & &
 \end{array}$$

Let $t := \gamma(t_1, t_2) \in F(X \times X)$, i.e., $d^{\downarrow F}(t_1, t_2) = \tilde{F}d(t) = 0$. Since we have a weak pullback, we observe that there exists $t' \in F\Delta_X$ with $Fe(t') = t$. (Since Fe is an embedding, t' and t actually coincide.) This implies that $t_1 = F\pi_1(t) = F\pi_1(Fe(t')) = F\pi_2(Fe(t')) = F\pi_2(t) = t_2$. \square

Apparently, Theorem 5.4.24 admits the following simple corollary.

Corollary 5.4.25 Let F be a weak pullback preserving endofunctor on \mathbf{Set} with well-behaved evaluation function ev_F and (X, d) be a metric space. If

the infimum in (5.4.1) is always a minimum then $d^{\downarrow F}$ is a metric and thus $\bar{F}(X, d) = (FX, d^{\downarrow F})$ is a metric space.

Please note that a similar restriction for the Kantorovich lifting (i.e., requiring that the supremum in Definition 5.4.4 is a maximum) does *not* yield preservation of metrics: In Example 5.4.10 the supremum is always a maximum but we do not get a metric. Let us now compare both lifting approaches.

Lemma 5.4.26 Let F be an endofunctor on Set with evaluation function ev_F and (X, d) be a pseudometric space. If ev_F satisfies Conditions W1 and W2 of Definition 5.4.14 then for all $t_1, t_2 \in FX$, all $t \in \Gamma_F(t_1, t_2)$ and all nonexpansive functions $f: (X, d) \rightarrow ([0, \top], d_e)$ we have $d_e(\tilde{F}f(t_1), \tilde{F}f(t_2)) \leq \tilde{F}d(t)$.

Proof. We have that $d_e \circ (f \times f) \leq d$ since f is nonexpansive. Now, due to monotonicity of the evaluation functor (Condition W1) we obtain $\tilde{F}d_e \circ F(f \times f) = \tilde{F}(d_e \circ (f \times f)) \leq \tilde{F}d$. Furthermore:

$$\begin{aligned} d_e(\tilde{F}f(t_1), \tilde{F}f(t_2)) &= d_e(\tilde{F}f(F\pi_1(t)), \tilde{F}f(F\pi_2(t))) = d_e(\tilde{F}(f \circ \pi_1)(t), \tilde{F}(f \circ \pi_2)(t)) \\ &= d_e(\tilde{F}(\pi_1 \circ (f \times f))(t), \tilde{F}(\pi_2 \circ (f \times f))(t)) \\ &= d_e(\tilde{F}\pi_1(F(f \times f)(t)), \tilde{F}\pi_2(F(f \times f)(t))) \\ &\leq \tilde{F}d_e(F(f \times f)(t)) = \tilde{F}(d_e \circ (f \times f))(t) \leq \tilde{F}d(t) \end{aligned}$$

where the first inequality is due to Condition W2, the second due to the above observation which was based on Condition W1. \square

Using this result we can see that under certain conditions the Wasserstein function is an upper bound for the Kantorovich pseudometric.

Theorem 5.4.27 (Comparison of the two Liftings) Let F be an endofunctor on Set . If ev_F satisfies Conditions W1 and W2 of Definition 5.4.14 then for all pseudometric spaces (X, d) we have $d^{\uparrow F} \leq d^{\downarrow F}$.

Proof. Let $t_1, t_2 \in FX$. We know (see the discussion after Definition 5.4.4) that a nonexpansive function $f: (X, d) \rightarrow ([0, \top], d_e)$ always exists but (see the discussion after Definition 5.4.12) couplings do not have to exist, so we have to distinguish two cases. If $\Gamma_F(t_1, t_2) = \emptyset$ we have $d^{\downarrow F}(t_1, t_2) = \top$ and clearly $d^{\uparrow F} \leq \top$. Otherwise we can apply Lemma 5.4.26 to obtain the desired inequality. \square

This inequality can be strict as the following example shows.

Example 5.4.28 (Wasserstein Lifting of the Squaring Functor) It is easy to see¹¹ that the squaring functor $S: \text{Set} \rightarrow \text{Set}$, $SX = X \times X$, $Sf = f \times f$ preserves weak pullbacks. We now first convince ourselves that the evaluation function $\text{ev}_S: S[0, \infty] \rightarrow [0, \infty]$, $\text{ev}_S(r_1, r_2) = r_1 + r_2$ given in Example 5.4.10 is well-behaved.

W1. Let $f, g: X \rightarrow [0, \infty]$ be given with $f \leq g$, then for all $t = (a, b) \in SX = X \times X$ we have $\tilde{S}f(t) = f(a) + f(b) \leq g(a) + g(b) = \tilde{S}g(t)$.

W2. For any $t = (r_1, r_2, r_3, r_4) \in S([0, \infty]^2)$ we have $\tilde{S}\pi_1(t) = r_1 + r_3$, $\tilde{S}\pi_2(t) = r_2 + r_4$ and $\tilde{S}d_e(t) = d_e(r_1, r_2) + d_e(r_3, r_4)$. We need to show the inequality $d_e(r_1 + r_3, r_2 + r_4) \leq d_e(r_1, r_2) + d_e(r_3, r_4)$. Apparently this is true if $r_1 + r_3 = r_2 + r_4$ so without loss of generality we assume $r_1 + r_3 < r_2 + r_4$ (the symmetrical case can be handled similarly). We distinguish two cases.

- ▷ Suppose $r_2 + r_4 = \infty$ then clearly $r_2 = \infty$ or $r_4 = \infty$ whereas $r_1, r_3 < \infty$. Thus we have $d(r_1, r_2) = \infty$ or $d(r_3, r_4) = \infty$ and hence also $d(r_1, r_2) + d(r_3, r_4) = \infty = d_e(r_1 + r_3, r_2 + r_4)$.
- ▷ Otherwise, if $r_2 + r_4 < \infty$ we have $r_1, r_2, r_3, r_4 < \infty$ and thus $d_e(r_1 + r_3, r_2 + r_4) = |r_1 + r_3 - r_2 - r_4| = |r_1 - r_2 + r_3 - r_4| \leq |r_1 - r_2| + |r_3 - r_4| = d_e(r_1, r_2) + d_e(r_3, r_4)$.

W3. Finally, $\text{ev}_S^{-1}[\{0\}] = \{(0, 0)\} = (i \times i)(\{0\} \times \{0\}) = \text{Si}[S\{0\}]$.

We now continue Example 5.4.10 where we considered a metric space (X, d) with at least two elements, chose an element $t_1 = (x_1, x_2) \in SX = X \times X$ with $x_1 \neq x_2$ and defined $t_2 = (x_2, x_1)$. The unique coupling $t \in \Gamma_S(t_1, t_2)$ is $t = ((x_1, x_2), (x_2, x_1))$. Using that d is a metric we conclude that $d^{\downarrow S}(t_1, t_2) = \tilde{S}d(t) = d(x_1, x_2) + d(x_2, x_1) = 2d(x_1, x_2) > 0$. However, in Example 5.4.10 we calculated $d^{\uparrow S}(t_1, t_2) = 0$.

Whenever the inequality in Theorem 5.4.27 can be replaced by an equality we will in the following say that the *Kantorovich-Rubinstein duality* or simply *duality* holds. In this case we obtain a canonical notion of distance on FX for any given pseudometric space (X, d) .

In order to show that the duality holds and simultaneously to calculate the distance of $t_1, t_2 \in FX$ it is enough to find a nonexpansive function $f: (X, d) \rightarrow ([0, \top], d_e)$ and a coupling $t \in \Gamma_F(t_1, t_2)$ such that $d_e(\tilde{F}f(t_1), \tilde{F}f(t_2)) =$

¹¹It also follows from the fact that the product bifunctor preserves weak pullbacks, which we will show later in Lemma 5.4.53.

$\tilde{F}d_e(t)$. Then, due to Theorem 5.4.27, this value equals $d^{\uparrow F}(t_1, t_2) = d^{\downarrow F}(t_1, t_2)$. We will often employ this technique for the upcoming examples.

Example 5.4.29 (Duality for the Identity Functor) We consider the identity functor Id with the identity function as evaluation function, i.e., $\text{ev}_{\text{Id}} = \text{id}_{[0, \top]}$. For any $t_1, t_2 \in X$, $t := (t_1, t_2)$ is the unique coupling of t_1, t_2 . Hence, $d^{\downarrow F}(t_1, t_2) = d(t_1, t_2)$. With the function $d(t_1, _): (X, d) \rightarrow ([0, \top], d_e)$, which is nonexpansive due to Lemma 5.2.9, we obtain duality because we have $d(t_1, t_2) = d_e(d(t_1, t_1), d(t_1, t_2)) \leq d^{\uparrow F}(t_1, t_2) \leq d^{\downarrow F}(t_1, t_2) = d(t_1, t_2)$ and thus equality. Similarly, if we define $\text{ev}_{\text{Id}}(r) = c \cdot r$ for $r \in [0, \top]$, $0 < c \leq 1$, the Kantorovich and Wasserstein liftings coincide and we obtain the discounted distance $d^{\uparrow F}(t_1, t_2) = d^{\downarrow F}(t_1, t_2) = c \cdot d(t_1, t_2)$.

Example 5.4.30 (Duality for the Distribution Functors) It is known that the probability distribution functor \mathcal{D} of Example 2.3.12 and its variants preserve weak pullbacks [Sok11, Proposition 3.3]. Let us now first show that the evaluation function $\text{ev}_{\mathcal{D}}: \mathcal{D}[0, 1] \rightarrow [0, 1]$, $\text{ev}_{\mathcal{D}}(P) = \mathbb{E}_P[\text{id}_{[0, 1]}] = \sum_{x \in [0, 1]} x \cdot P(x)$ which we have defined in Example 5.4.9 is well-behaved for all variants of the distribution functor (i.e., distributions and subdistributions with countable or finite supports).

W1. This is just the monotonicity of the expected value. For $f, g: X \rightarrow [0, 1]$ with $f \leq g$ and any (sub)probability distribution $P: X \rightarrow [0, 1]$ we have

$$\tilde{F}f(P) = \sum_{x \in X} f(x) \cdot P(x) \leq \sum_{x \in X} g(x) \cdot P(x) = \tilde{F}g(P).$$

W2. In order to prove Condition W2 we assume any probability or subprobability distribution $P: [0, 1]^2 \rightarrow [0, 1]$ and calculate

$$\begin{aligned} d_e(\tilde{\mathcal{D}}\pi_1(P), \tilde{\mathcal{D}}\pi_2(P)) &= |\mathbb{E}_P[\pi_1] - \mathbb{E}_P[\pi_2]| = \left| \sum_{x_1, x_2 \in [0, 1]} (x_1 - x_2) \cdot P(x_1, x_2) \right| \\ &\leq \sum_{x_1, x_2 \in [0, 1]} |x_1 - x_2| \cdot P(x_1, x_2) \\ &= \sum_{x_1, x_2 \in [0, 1]} d_e(x_1, x_2) \cdot P(x_1, x_2) = \mathbb{E}_P[d_e] = \tilde{\mathcal{D}}d_e(P). \end{aligned}$$

W3. Let us first assume we are dealing with proper probability distributions, not subdistributions. We denote for any set X with $0 \in X$, by $\delta_0^X \in \mathcal{D}X$ the Dirac distribution $\delta_0^X: X \rightarrow [0, 1]$ with $\delta_0^X(0) = 1$ and $\delta_0^X(x) = 0$ for

$x \in X \setminus \{0\}$. We observe that $\mathcal{D}\{0\} = \{\delta_0^{\{0\}}\}$ and thus we can easily see that also Condition W₃ holds: $\text{ev}_{\mathcal{D}}^{-1}[\{0\}] = \{\delta_0^{\{0,1\}}\} = \mathcal{Di}[\mathcal{D}\{0\}]$.

If we consider subprobability distributions, we have $\mathcal{D}\{0\} = [0, 1]^{\{0\}}$ and $\text{ev}_{\mathcal{D}}^{-1}[\{0\}] = \{P: [0, 1] \rightarrow [0, 1] \mid \forall x \in]0, 1]. P(x) = 0\} = \mathcal{Di}[\mathcal{D}\{0\}]$ which concludes the proof of Condition W₃.

With this well-behaved evaluation function we thus recover the usual Wasserstein pseudometric, i.e., for any (sub)probability distributions $P_1, P_2: X \rightarrow [0, 1]$ we have

$$d^{\downarrow \mathcal{D}}(P_1, P_2) = \inf \left\{ \sum_{x_1, x_2 \in X} d(x_1, x_2) \cdot P(x_1, x_2) \mid P \in \Gamma_{\mathcal{D}}(P_1, P_2) \right\}$$

and – for proper distributions only – the Kantorovich-Rubinstein duality [Vil09] from transportation theory for the discrete case. Moreover, in this case it is easy to see that for finite supports the above infimum is always a minimum: Let $\text{supp}(P_1) \cup \text{supp}(P_2) = \{s_1, \dots, s_n\}$ be the union of the finite supports of P_1 and P_2 . We define the following finitely many real numbers $p_{1i} := P_1(s_i)$, $p_{2j} := P_2(s_j)$, $d_{ij} := d(s_i, s_j)$. Then the distance of P_1 and P_2 can be equivalently expressed as the following linear program:

$$\begin{aligned} & \text{minimize} && \sum_{1 \leq i, j \leq n} d_{ij} \cdot x_{ij} \\ & \text{subject to} && \sum_{1 \leq j \leq n} x_{ij} = p_{1i}, \quad 1 \leq i \leq n \\ & && \sum_{1 \leq i \leq n} x_{ij} = p_{2j}, \quad 1 \leq j \leq n \\ & && 0 \leq x_{ij} \leq 1, \quad 1 \leq i, j \leq n \end{aligned}$$

The feasible region is nonempty ($x_{ij} := p_{1i} \cdot p_{2j}$ is in it) and bounded. Thus we indeed get an optimal solution x_{ij}^* and can define the optimal coupling as $P^*(s_i, s_j) := x_{ij}^*$.

In the case of subdistributions we do not have duality: Let $P, Q: \mathbb{1} \rightarrow [0, 1]$ be subdistributions on the singleton set $\mathbb{1}$, i.e., $P(\checkmark) = p$ and $Q(\checkmark) = q$ with $p, q \in [0, 1]$. The only pseudometric on $\mathbb{1}$ is the discrete metric d so any function $f: \mathbb{1} \rightarrow [0, 1]$ is nonexpansive and we have $\tilde{\mathcal{D}}f(P) = f(\checkmark) \cdot P(\checkmark)$. Hence the Kantorovich distance of P and Q is achieved for the function f where $f(\checkmark) = 1$ and equals $d^{\uparrow F}(P, Q) = |p - q|$. However, if $p \neq q$ it is easy to see that there are no couplings of P and Q so $d^{\downarrow F}(P, Q) = 1$. Thus for any p, q where $|p - q| < 1$ we do not have equality.

Example 5.4.31 (The Hausdorff Pseudometric for Finite Sets) Similar to Example 5.4.16 we assume $\top = \infty$ but here we just consider the finite powerset functor \mathcal{P}_f with evaluation function $\max: \mathcal{P}_f([0, \infty]) \rightarrow [0, \infty]$ with $\max \emptyset = 0$. We claim that in this setting we obtain duality and both pseudometrics are equal to the *Hausdorff pseudometric* d_H on $\mathcal{P}_f(X)$ which is defined as, for all $X_1, X_2 \in \mathcal{P}_f X$,

$$d_H(X_1, X_2) = \max \left\{ \max_{x_1 \in X_1} \min_{x_2 \in X_2} d(x_1, x_2), \max_{x_2 \in X_2} \min_{x_1 \in X_1} d(x_1, x_2) \right\}.$$

Note that this distance is ∞ , if either X_1 or X_2 is empty.

We show our claim by proving that if X_1, X_2 are both non-empty there exists a coupling and a nonexpansive function that both witness the Hausdorff distance. Assume that the first value $\max_{x_1 \in X_1} \min_{x_2 \in X_2} d(x_1, x_2)$ is maximal and assume that $y_1 \in X_1$ is the element of X_1 for which the maximum is reached. Furthermore let $y_2 \in X_2$ be the closest element in X_2 , i.e., the element for which $d(y_1, y_2)$ is minimal. We know that for all $x_1 \in X_1$ there exists $x_2^{x_1}$ such that $d(x_1, x_2^{x_1}) \leq d(y_1, y_2)$ and for all $x_2 \in X_2$ there exists $x_1^{x_2}$ such that $d(x_1^{x_2}, x_2) \leq d(y_1, y_2)$. Specifically, $x_2^{y_1} = y_2$. We use the coupling $T \subseteq X \times X$ with

$$T = \{(x_1, x_2^{x_1}) \mid x_1 \in X_1\} \cup \{(x_1^{x_2}, x_2) \mid x_2 \in X_2\}.$$

Indeed, we obviously have $\mathcal{P}_f \pi_i(T) = X_i$ and $\mathcal{P}_f d(T)$ contains all distances between the elements above, of which the distance $d(y_1, y_2) = d^H(X_1, X_2)$ is maximal. We now define a nonexpansive function $f: (X, d) \rightarrow ([0, \top], d_e)$ as follows: $f(x) = \min_{x_2 \in X_2} d(x, x_2)$. It holds that

$$\max \mathcal{P}_f f(X_1) = \max f[X_1] = \max_{x_1 \in X_1} \min_{x_2 \in X_2} d(x_1, x_2) = d^H(X_1, X_2)$$

and $\max \mathcal{P}_f f(X_2) = \max f[X_2] = 0$. Hence, the difference of both values is $d^H(X_1, X_2)$. It remains to show that f is nonexpansive. Let $x, y \in X$ and let $x_2, y_2 \in X_2$ be elements for which the distances $d(x, x_2), d(y, y_2)$ are minimal. Hence

$$\begin{aligned} d(x, x_2) &\leq d(x, y_2) \leq d(x, y) + d(y, y_2) \\ \wedge \quad d(y, y_2) &\leq d(y, x_2) \leq d(y, x) + d(x, x_2). \end{aligned}$$

Lemma 5.2.2 implies that $d(x, y) \geq d_e(d(x, x_2), d(y, y_2)) = d_e(f(x), f(y))$.

If $X_1 = X_2 = \emptyset$, we can use the coupling $T = \emptyset = \emptyset \times \emptyset$ and any function f . If, instead $X_1 = \emptyset, X_2 \neq \emptyset$, no coupling exists thus $d^{\downarrow F} = \infty$ and we can take the constant ∞ -function to show that also $d^{\uparrow F} = \infty$ is attained.

To illustrate the Hausdorff pseudometric, we quickly provide the example calculation which yields the distance given in Example 5.3.3 (page 142).

Example 5.4.32 For the set of real numbers we take the usual Euclidean distance and want to compute the Hausdorff distance between the set $\{0.4, 0.7\}$ and the set $\{0.5, 1\}$. Here we have

$$\begin{aligned} \max_{x_1 \in \{0.4, 0.7\}} \min_{x_2 \in \{0.5, 1\}} |x_1 - x_2| &= \max \{ \min \{0.1, 0.6\}, \min \{0.2, 0.3\} \} \\ &= \max \{0.1, 0.2\} = 0.2 \end{aligned}$$

and similarly

$$\begin{aligned} \max_{x_2 \in \{0.5, 1\}} \min_{x_1 \in \{0.4, 0.7\}} |x_1 - x_2| &= \max \{ \min \{0.1, 0.2\}, \min \{0.6, 0.3\} \} \\ &= \max \{0.1, 0.3\} = 0.3 \end{aligned}$$

resulting in $d_H(\{0.5, 1\}, \{0.4, 0.7\}) = \max \{0.2, 0.3\} = 0.3$ as claimed in Example 5.3.3 (page 142).

It would also be interesting to consider the countable powerset functor, use the supremum as (well-behaved) evaluation function and consider the resulting Wasserstein lifting. However, in this case we cannot use the same proof technique as above because the Hausdorff pseudometric for countable sets (with supremum/infimum replacing maximum/minimum) does not preserve metrics. If we take the Euclidean metric and consider the sets $X_1 = \{0\} \cup \{1/n \mid n \in \mathbb{N}\}$ and $X_2 = \{1/n \mid n \in \mathbb{N}\}$ then their Hausdorff distance is 0 although clearly X_1 and X_2 are different sets. Thus, due to Theorem 5.4.24 (Page 161), there cannot be an optimal coupling for X_1 and X_2 .

As another example of our lifting approaches, we consider the input functor $_{-}^{\Lambda}$ of Example 2.4.2. It is known that the input functor even preserves pullbacks [Rutoo]. Nevertheless we provide a proof here.

Lemma 5.4.33 Let A be an arbitrary set. The input functor $_{-}^{\Lambda}: \text{Set} \rightarrow \text{Set}$ of Example 2.4.2 preserves pullbacks.

Proof. We look at the following diagram.

$$\begin{array}{ccc} P & \xrightarrow{p_1} & X_1 \\ p_2 \downarrow & & \downarrow f_1 \\ X_2 & \xrightarrow{f_2} & Y \end{array} \qquad \begin{array}{ccc} P^{\Lambda} & \xrightarrow{p_1^{\Lambda}} & X_1^{\Lambda} \\ p_2^{\Lambda} \downarrow & & \downarrow f_1^{\Lambda} \\ X_2^{\Lambda} & \xrightarrow{f_2^{\Lambda}} & Y^{\Lambda} \end{array}$$

If we have a pullback in Set as indicated in the left part of the diagram, we have to show that also the right diagram is a pullback. The diagram on the right commutes because for all $g \in P^A$ we know from the commutativity of the left diagram that $f_1^A \circ p_1^A(g) = f_1 \circ p_1 \circ g = f_2 \circ p_2 \circ g = f_2^A \circ p_2^A(g)$. Moreover, if Q is a set along with functions $q_i: Q \rightarrow X_i^A$ satisfying $f_1^A \circ q_1 = f_2^A \circ q_2$, for each $a \in A$ the induced functions $q_i(\cdot)(a): Q \rightarrow X_i$ satisfy $f_1 \circ q_1(\cdot)(a) = f_2 \circ q_2(\cdot)(a)$. Thus, since the left diagram is a pullback, for each $a \in A$ there is a unique function $f_a: Q \rightarrow P$ such that $p_i \circ f_a = q_i(\cdot)(a)$. We define $f: Q \rightarrow P^A$ via the assignment $f(q)(a) := f_a(q)$. Then we have $p_i^A \circ f(q)(a) = p_i \circ f_a(q) = q_i(q)(a)$ for all $q \in Q$ and all $a \in A$ and thus $p_i^A \circ f = q_i$. Moreover, this is the only function satisfying these equalities. Any $f': Q \rightarrow P^A$ which satisfies them induces functions $f'_a: Q \rightarrow P$ via the assignment $f'_a(q) := f'(q)(a)$ and each of these must be equal to the unique function f_a and thus $f' = f$. \square

For the input functor we will consider two different well-behaved evaluation functions and the resulting Wasserstein pseudometrics.

Example 5.4.34 (Wasserstein Lifting for the Input Functor) We consider the input functor $_{-}^A: \text{Set} \rightarrow \text{Set}$ of Example 2.4.2 with finite input set A and claim that the evaluation functions $\text{ev}_F: [0, \top]^A \rightarrow [0, \top]$ which are listed in the table below are well-behaved and yield the given Wasserstein pseudometric on X^A for any pseudometric space (X, d) .

maximal distance \top	$\text{ev}_F(s)$	$d^{\downarrow F}(s_1, s_2)$
$\top \in]0, \infty]$	$\max_{a \in A} s(a)$	$\max_{a \in A} d(s_1(a), s_2(a))$
$\top = \infty$	$\sum_{a \in A} s(a)$	$\sum_{a \in A} d(s_1(a), s_2(a))$
$\top \in]0, \infty[$	$ A ^{-1} \sum_{a \in A} s(a)$	$ A ^{-1} \sum_{a \in A} d(s_1(a), s_2(a))$

In order to show this we first observe that for any $f: X \rightarrow [0, \top]$ we have $\tilde{F}f = \text{ev}_F \circ f^A$ so applying it to $s \in X^A$ yields either $\max_{a \in A} f(s(a))$ or $\sum_{a \in A} f(s(a))$ or $|A|^{-1} \sum_{a \in A} f(s(a))$. With this we proceed to show well-behavedness.

W1. For $f_1, f_2: X \rightarrow [0, \top]$ with $f_1 \leq f_2$ we obviously also have $\tilde{F}f_1 \leq \tilde{F}f_2$.

W2. Let $s \in ([0, \top]^2)^A$ and $s_i := \pi_i^A(t)$, i.e., necessarily $s = \langle s_1, s_2 \rangle$. We have to show the inequality $d_e(\text{ev}_F(s_1), \text{ev}_F(s_2)) \leq \tilde{F}d_e(s)$ where the right hand side evaluates to $\text{ev}_F(d_e^A(s)) = \text{ev}_F(d_e \circ s) = \text{ev}_F(d_e \circ \langle s_1, s_2 \rangle)$. Using this we can see that the inequality is an immediate consequence of Lemma 5.2.3 (page 136) by taking $f = s_1$, $g = s_2$ or, in the last case, $f = |A|^{-1}s_1$ and $g = |A|^{-1}s_2$.

W3. We have $\text{ev}_F^{-1}[\{0\}] = \{s: A \rightarrow [0, \top] \mid \text{ev}_F(s) = 0\}$. Clearly for all functions this is the case only if s is the constant 0-function. Since $\{0\}$ is a final object in Set , there is a unique function $z: A \rightarrow \{0\}$. Thus $\text{Fi}[F\{0\}] = i^A[\{0\}^A] = \{i^A(z)\} = \{i \circ z\}$ and clearly $i \circ z: A \rightarrow [0, \top]$ is also the constant 0-function.

Now if we have $s_1, s_2 \in X^A$ their unique coupling is $s := \langle s_1, s_2 \rangle: A \rightarrow X \times X$. Moreover $\widetilde{\text{Fd}}(s) = \text{ev}_F(d^A(s)) = \text{ev}_F(d \circ \langle s_1, s_2 \rangle)$ and using the different evaluation functions we obtain the pseudometrics given in the table above.

Finally, using a similar argument as in Example 5.4.28, we can show that the duality does not hold: Suppose both X and A have more than one element and d is a metric on X . Let $s_1 \in X^A$ such that there are a_1, a_2 with $s_1(a_1) \neq s_1(a_2)$. We define $s_2(a_1) = s_1(a_2)$, $s_2(a_2) = s_1(a_1)$ and $s_2(a) = s_1(a)$ for all remaining $a \in A \setminus \{a_1, a_2\}$. Clearly $s_1 \neq s_2$ but $\widetilde{\text{Ff}}(s_1) = \widetilde{\text{Ff}}(s_2)$ for every nonexpansive function $f: (X, d) \rightarrow ([0, \top], d_e)$ yielding $d^{\uparrow F}(s_1, s_2) = 0$ whereas $d^{\downarrow F}(s_1, s_2) > 0$ since $d^{\downarrow F}$ is a metric by Theorem 5.4.24 (page 161).

We conclude our list of examples with the Wasserstein lifting of the machine functor which we will use several times in the remainder of this chapter.

Example 5.4.35 (Wasserstein Lifting of the Machine Functor) We equip the machine functor $M_B = B \times _^A$ with the evaluation function $\text{ev}_{M_B}: B \times [0, \top]^A \rightarrow [0, \top]$, $(o, s) \mapsto c \cdot \text{ev}_I(s)$ where $c \in]0, 1]$ is a discount factor and ev_I is one of the evaluation functions for the input functor from Example 5.4.34. For any pseudometric space (X, d) we can easily see that for two elements $(o_1, s_1), (o_2, s_2) \in B \times X^A$ we have a unique coupling if and only if $o_1 = o_2$, namely $(o_1, \langle s_1, s_2 \rangle)$ (for $o_1 \neq o_2$ no coupling exists at all). Thus the Wasserstein function on any two elements as above is given by

$$d^{\downarrow M_2}((o_1, s_1), (o_2, s_2)) = \begin{cases} 1, & \text{if } o_1 \neq o_2 \\ c \cdot \text{ev}_I(d \circ \langle s_1, s_2 \rangle), & \text{else} \end{cases}$$

where the latter is either $c \cdot \max_{a \in A} d(s_1(a), s_2(a))$ or $\sum_{a \in A} d(s_1(a), s_2(a))$ depending on the choice of ev_I .

5.4.3 Lifting Multifunctors

While the functors we considered so far can be nicely lifted using our theory, there are other functors that require a more general treatment. For instance, consider the output functor $F = B \times _$ for some fixed set B (see Example 2.4.3, page 50). As in Example 5.4.35 we have a coupling for $t_1, t_2 \in FX = B \times X$ with $t_i = (b_i, x_i)$ if and only if $b_1 = b_2$. Consequently, if $b_1 \neq b_2$ then irrespective

of the evaluation function we choose and of the distance between x_1 and x_2 in (X, d) , the lifted Wasserstein pseudometric will always result in $d^{\downarrow F}(t_1, t_2) = \top$. This can be counterintuitive, e.g., taking $B = [0, 1]$, $X \neq \emptyset$ and $t_1 = (0, x)$ and $t_2 = (\varepsilon, x)$ for a small $\varepsilon > 0$ and an $x \in X$. The reason is that we think of $B = [0, 1]$ as if it were endowed with a non-discrete pseudometric, like e.g. the Euclidean metric d_e , plugged into the product after the lifting.

This intuition can be formalized by considering the lifting of the product seen as a functor from $\text{Set} \times \text{Set}$ into Set . More generally, it can be seen that the definitions and results introduced so far for endofunctors in Set straightforwardly extend to multifunctors on Set , i.e., to functors $F: \text{Set}^n \rightarrow \text{Set}$ on the product category Set^n for any natural number $n \in \mathbb{N}$. The only difference is that we start with n pseudometric spaces instead of one. Due to this, the definitions and results are technically a bit more complicated than in the endofunctor setting but they capture exactly the same ideas as before.

For clarity we provide all the multifunctor results here but it is safe to skip the results at a first read, continue with studying the product and coproduct bifunctors in Section 5.4.4 (page 175) – they will play an important role for the later development of our theory – and only look at the exact multifunctor definitions when necessary.

The formal definition of multifunctor lifting is a straightforward extension of Definition 5.4.1 with only a little bit of added technical complexity.

Definition 5.4.36 (Lifting of a Multifunctor) Let $U: \text{PMet} \rightarrow \text{Set}$ be the forgetful functor which maps every pseudometric space to its underlying set and denote by $U^n: \text{PMet}^n \rightarrow \text{Set}^n$ the n -fold product of U with itself, i.e., the functor mapping the product of n pseudometric spaces to the product of their base sets. A functor $\bar{F}: \text{PMet}^n \rightarrow \text{PMet}$ is called a *lifting* of a functor $F: \text{Set}^n \rightarrow \text{Set}$ if it satisfies $U \circ \bar{F} = F \circ U^n$.

We quickly note that these multifunctor liftings can be used to obtain endofunctor liftings.

Lemma 5.4.37 (Multifunctor Lifting Induces Endofunctor Lifting) Let $n \in \mathbb{N}$, $n \geq 2$ and $i \in \{1, \dots, n\}$. Moreover, let $\bar{F}: \text{PMet}^n \rightarrow \text{PMet}$ be a lifting of a functor $F: \text{Set}^n \rightarrow \text{Set}$. If we fix all but the i -th component and consider the endofunctor $\bar{F}_i: \text{PMet} \rightarrow \text{PMet}$ where

$$\begin{aligned} \bar{F}_i(X, d) &:= \bar{F}((X_1, d_1), \dots, (X_{i-1}, d_{i-1}), (X, d), (X_{i+1}, d_{i+1}), \dots, (X_n, d_n)) \\ \bar{F}_i f &:= \bar{F}(\text{id}_{X_1}, \dots, \text{id}_{X_{i-1}}, f, \text{id}_{X_{i+1}}, \dots, \text{id}_{X_n}) \end{aligned}$$

then this is a lifting of the endofunctor $F_i: \text{Set} \rightarrow \text{Set}$, where

$$\begin{aligned} F_i X &:= F(X_1, \dots, X_{i-1}, X, X_{i+1}, \dots, X_n), \\ F_i f &:= F(\text{id}_{X_1}, \dots, \text{id}_{X_{i-1}}, f, \text{id}_{X_{i+1}}, \dots, \text{id}_{X_n}), \end{aligned}$$

in the sense of Definition 5.4.1.

Proof. We just have to use the property $U \circ \bar{F} = F \circ U^n$ to obtain

$$\begin{aligned} U \circ \bar{F}_i(X, d) &= U \circ \bar{F}((X_1, d_1), \dots, (X_{i-1}, d_{i-1}), (X, d), (X_{i+1}, d_{i+1}), \dots, (X_n, d_n)) \\ &= F \circ U^n((X_1, d_1), \dots, (X_{i-1}, d_{i-1}), (X, d), (X_{i+1}, d_{i+1}), \dots, (X_n, d_n)) \\ &= F(X_1, \dots, X_{i-1}, X, X_{i+1}, \dots, X_n) = F_i \circ U(X, d) \end{aligned}$$

for any pseudometric space (X, d) . Completely analogously one can prove that this equality holds for arrows which yields $U \circ \bar{F}_i = F_i \circ U$. \square

As in the endofunctor case any multifunctor lifting is monotone in the following sense.

Theorem 5.4.38 (Monotonicity of Multifunctor Lifting) Let $F: \text{Set}^n \rightarrow \text{Set}$ be a multifunctor and $\bar{F}: \text{PMet}^n \rightarrow \text{PMet}$ be a lifting of F . For pseudometric spaces $(X_1, d_1), \dots, (X_n, d_n)$ let $(d_1, \dots, d_n)^F$ denote the pseudometric on $F(X_1, \dots, X_n)$ which we obtain by applying \bar{F} to $(X_1, d_1), \dots, (X_n, d_n)$. Then \bar{F} is monotone on pseudometrics in the following sense: If we have pseudometrics $d_i \leq e_i$ on common sets X_i we also have $(d_1, \dots, d_n)^F \leq (e_1, \dots, e_n)^F$.

Proof. Since for all $i \in \{1, \dots, n\}$ we have $d_i \leq e_i$ the identity function $\text{id}_i := \text{id}_{X_i}: X_i \rightarrow X_i$ can be regarded as a nonexpansive function $f_i: (X, e_i) \rightarrow (X, d_i)$ because we have for all $x, y \in X_i$ that

$$d_i(f_i(x), f_i(y)) = d_i(x, y) \leq e_i(x, y).$$

By functoriality of \bar{F} also

$$\bar{F}(f_1, \dots, f_n): (F(X_1, \dots, X_n), (e_1, \dots, e_n)^F) \rightarrow (F(X_1, \dots, X_n), (d_1, \dots, d_n)^F)$$

is nonexpansive, i.e., for all $t_1, t_2 \in F(X_1, \dots, X_n)$ we have

$$(d_1, \dots, d_n)^F(F(Uf_1, \dots, Uf_n)(t_1), F(Uf_1, \dots, Uf_n)(t_2)) \leq (e_1, \dots, e_n)^F(t_1, t_2)$$

and the left hand side evaluates to

$$\begin{aligned} &(d_1, \dots, d_n)^F(F(Uf_1, \dots, Uf_n)(t_1), F(Uf_1, \dots, Uf_n)(t_2)) \\ &= (d_1, \dots, d_n)^F(F(\text{id}_1, \dots, \text{id}_n)(t_1), F(\text{id}_1, \dots, \text{id}_n)(t_2)) \\ &= (d_1, \dots, d_n)^F(\text{id}_{F(X_1, \dots, X_n)}(t_1), \text{id}_{F(X_1, \dots, X_n)}(t_2)) \\ &= (d_1, \dots, d_n)^F(t_1, t_2) \end{aligned}$$

and thus we have indeed $(d_1, \dots, d_n)^F \leq (e_1, \dots, e_n)^F$. \square

It is not too surprising that the line of argument in the above proof is exactly the same as used in the proof of Theorem 5.4.2 (page 144). One just has to take proper care of putting the universal quantification (for all $1 \leq i \leq n$) in the right place. Thus for many of the following theorems there will be just a reference to the corresponding endofunctor result and the simple (but admittedly tedious) calculations are omitted.

The really useful feature of considering multifunctor liftings is based on the fact that we have a slightly different domain of definition for evaluation functions which will also help us to solve the problems we described initially.

Definition 5.4.39 (Multifunctor Evaluation Function and Evaluation Functor)

Let $F: \text{Set}^n \rightarrow \text{Set}$ be a functor. An *evaluation function* for F is any function

$$\text{ev}_F: F([0, \top], \dots, [0, \top]) \rightarrow [0, \top].$$

Given such an evaluation function, the *evaluation functor* is the functor

$$\tilde{F}: (\text{Set}/[0, \top])^n \rightarrow \text{Set}/[0, \top]$$

where $\tilde{F}(g_1, \dots, g_n) := \text{ev}_F \circ F(g_1, \dots, g_n)$ for all $g_i \in \text{Set}/[0, \top]$ and on arrows \tilde{F} coincides with F .

Using this function, we immediately get the Kantorovich pseudometric and the corresponding lifting.

Definition 5.4.40 (Kantorovich Function for Multifunctors) Let $F: \text{Set}^n \rightarrow \text{Set}$ be a functor with evaluation function $\text{ev}_F: F([0, \top], \dots, [0, \top]) \rightarrow [0, \top]$ and $(X_1, d_1), \dots, (X_n, d_n)$ be pseudometric spaces. The *Kantorovich function* is the function $(d_1, \dots, d_n)^{\uparrow F}: (F(X_1, \dots, X_n))^2 \rightarrow [0, \top]$, where

$$(d_1, \dots, d_n)^{\uparrow F}(t_1, t_2) := \sup_{f_i: (X_i, d_i) \rightarrow ([0, \top], d_e)} d_e\left(\tilde{F}(f_1, \dots, f_n)(t_1), \tilde{F}(f_1, \dots, f_n)(t_2)\right)$$

for all $t_1, t_2 \in F(X_1, \dots, X_n)$.

By adapting the proof of Theorem 5.4.5 (page 145) we immediately obtain.

Theorem 5.4.41 For all pseudometric spaces $(X_1, d_1), \dots, (X_n, d_n)$ the Kantorovich function $(d_1, \dots, d_n)^{\uparrow F}$ is a pseudometric on $F(X_1, \dots, X_n)$.

Thus we can define the Kantorovich lifting as follows.

Definition 5.4.42 (Kantorovich Lifting for Multifunctors) Let $F: \text{Set}^n \rightarrow \text{Set}$ be a functor with evaluation function $\text{ev}_F: F([0, \top], \dots, [0, \top]) \rightarrow [0, \top]$. The *Kantorovich lifting* of F is the functor $\bar{F}: \text{PMet}^n \rightarrow \text{PMet}$, $\bar{F}((X_1, d_1), \dots, (X_n, d_n)) = (F(X_1, \dots, X_n), d)$ with the pseudometric $d = (d_1, \dots, d_n)^{\uparrow F}$, and $\bar{F}f = Ff$.

By adapting the proof of Theorem 5.4.7 (page 146) we can guarantee the soundness of this definition.

Theorem 5.4.43 The Kantorovich lifting is a functor $\text{PMet}^n \rightarrow \text{PMet}$.

Also the Wasserstein lifting can be transferred to the multifunctor setting. For this we first need to define couplings.

Definition 5.4.44 (Coupling) Let $F: \text{Set}^n \rightarrow \text{Set}$ be a functor and $m \in \mathbb{N}$. Given sets X_1, \dots, X_n and elements $t_j \in F(X_1, \dots, X_n)$ for $1 \leq j \leq m$ we call an element $t \in F(X_1^m, \dots, X_n^m)$ such that $F(\pi_{1,j}, \dots, \pi_{n,j})(t) = t_j$ a *coupling* of the t_j (with respect to F) where $\pi_{i,j}$ are the projections $\pi_{i,j}: X_i^m \rightarrow X_i$. We write $\Gamma_F(t_1, t_2, \dots, t_m)$ for the set of all these couplings.

Using these couplings we can then again define a Wasserstein function.

Definition 5.4.45 (Wasserstein Function for Multifunctors) Let $F: \text{Set}^n \rightarrow \text{Set}$ be a functor with evaluation function $\text{ev}_F: F([0, \top], \dots, [0, \top]) \rightarrow [0, \top]$ and $(X_1, d_1), \dots, (X_n, d_n)$ be pseudometric spaces. The *Wasserstein function* is the function $(d_1, \dots, d_n)^{\downarrow F}: (F(X_1, \dots, X_n))^2 \rightarrow [0, \top]$, where

$$(d_1, \dots, d_n)^{\downarrow F}(t_1, t_2) := \inf_{t \in \Gamma_F(t_1, t_2)} \tilde{F}(d_1, \dots, d_n)(t).$$

for all $t_1, t_2 \in F(X_1, \dots, X_n)$.

As before, we will use well-behaved evaluation functions along with pullback preserving functors to obtain a Wasserstein pseudometric.

Definition 5.4.46 (Well-Behaved Multifunctor Evaluation Function) We call a multifunctor evaluation function $\text{ev}_F: F([0, \top], \dots, [0, \top]) \rightarrow [0, \top]$ *well-behaved* if it satisfies the following three properties.

W1. \tilde{F} is monotone, i.e., given $f_i, g_i: X_i \rightarrow [0, \top]$ with $f_i \leq g_i$ for all $1 \leq i \leq n$, we also have $\tilde{F}(f_1, \dots, f_n) \leq \tilde{F}(g_1, \dots, g_n)$.

W2. Let $\pi_i: [0, \top]^2 \rightarrow [0, \top]$ be the projections of the product. For all couplings

$t \in F([0, \top]^2, \dots, [0, \top]^2)$ we require

$$d_e\left(\tilde{F}(\pi_1, \dots, \pi_1)(t), \tilde{F}(\pi_2, \dots, \pi_2)(t)\right) \leq \tilde{F}(d_e, \dots, d_e)(t).$$

W₃. We have $\text{ev}_F^{-1}[\{0\}] = F(i, \dots, i)[F(\{0\}, \dots, \{0\})]$ where $i: \{0\} \hookrightarrow [0, \top]$ is the inclusion map.

Of course, also the Gluing Lemma, Lemma 5.4.18, has a natural generalization to multifunctors.

Lemma 5.4.47 (Gluing Lemma for Multifunctors) Let $F: \text{Set}^n \rightarrow \text{Set}$ be a weak pullback preserving multifunctor, X_1, \dots, X_n be sets, $t_1, t_2, t_3 \in F(X_1, \dots, X_n)$, $t_{12} \in \Gamma_F(t_1, t_2)$ and $t_{23} \in \Gamma_F(t_2, t_3)$ be couplings. For $i \in \{1, \dots, n\}$ and $j \in \{1, 2, 3\}$ we denote by $\pi_{i,j}: X_i^3 \rightarrow X_i$ the projections of the respective ternary products.

There exists a coupling $t_{123} \in \Gamma_F(t_1, t_2, t_3)$ such that

$$\begin{aligned} F(\langle \pi_{1,1}, \pi_{1,2} \rangle, \dots, \langle \pi_{n,1}, \pi_{n,2} \rangle)(t_{123}) &= t_{12}, \text{ and} \\ F(\langle \pi_{1,2}, \pi_{1,3} \rangle, \dots, \langle \pi_{n,2}, \pi_{n,3} \rangle)(t_{123}) &= t_{23}. \end{aligned}$$

Moreover, $t_{13} := F(\langle \pi_{1,1}, \pi_{1,3} \rangle, \dots, \langle \pi_{n,1}, \pi_{n,3} \rangle)(t_{123})$ is a coupling of t_1 and t_3 , i.e., we have $t_{13} \in \Gamma_F(t_1, t_3)$.

Using this lemma and well-behavedness we can prove sufficient conditions for the Wasserstein function to be a pseudometric just as we did in Theorem 5.4.20.

Theorem 5.4.48 Let $F: \text{Set}^n \rightarrow \text{Set}$ be a functor with evaluation function ev_F . If

1. F preserves weak pullbacks and
2. ev_F is well-behaved

then the Wasserstein function is a pseudometric.

This result then gives rise to the Wasserstein lifting for multifunctors.

Definition 5.4.49 (Wasserstein Lifting for Multifunctors) Let $F: \text{Set}^n \rightarrow \text{Set}$ be a weak pullback preserving functor with well-behaved evaluation function $\text{ev}_F: F([0, \top], \dots, [0, \top]) \rightarrow [0, \top]$. We define the *Wasserstein lifting* of the functor F to be the functor $\bar{F}: \text{PMet}^n \rightarrow \text{PMet}$, $\bar{F}((X_1, d_1), \dots, (X_n, d_n)) = (F(X_1, \dots, X_n), d)$ with the pseudometric $d = (d_1, \dots, d_n)^{\downarrow F}$ and $\bar{F}f = Ff$.

This definition is justified by adapting the proof of Theorem 5.4.22 (page 158) to obtain the following result.

Lemma 5.4.50 The Wasserstein lifting is a functor $\text{PMet}^n \rightarrow \text{PMet}$.

With these results at hand we quickly summarize a few of the properties for the multifunctor liftings which arise as natural generalizations of Lemma 5.4.26 and theorems 5.4.8, 5.4.23, 5.4.24 and 5.4.27.

Theorem 5.4.51 Let $F: \text{Set}^n \rightarrow \text{Set}$ be a functor with evaluation function ev_F .

1. Both liftings preserve isometries.
2. If the evaluation function satisfies Conditions W1 and W2 of Definition 5.4.46 then $(d_1, \dots, d_n)^{\uparrow F} \leq (d_1, \dots, d_n)^{\downarrow F}$ holds for all pseudometric spaces (X_i, d_i) .
3. If F preserves weak pullbacks, ev_F is well-behaved and for all $t_1, t_2 \in F(X_1, \dots, X_n)$ with $(d_1, \dots, d_n)^{\downarrow F}(t_1, t_2) = 0$ there is an optimal coupling $\gamma(t_1, t_2) \in \Gamma_F(t_1, t_2)$ s.t. $0 = (d_1, \dots, d_n)^{\downarrow F}(t_1, t_2) = \tilde{F}(d_1, \dots, d_n)(\gamma(t_1, t_2))$ then $(d_1, \dots, d_n)^{\downarrow F}$ is a metric for all metric spaces (X_i, d_i) .

Whenever the two pseudometrics coincide for a functor and an evaluation function, we say that the *Kantorovich-Rubinstein duality* or short *duality* holds.

5.4.4 The Product and Coproduct Bifunctors

We conclude our section on multifunctors by considering two important examples in length, the product and the coproduct bifunctor.

Definition 5.4.52 (Product Bifunctor) The *product bifunctor* is the bifunctor $F: \text{Set}^2 \rightarrow \text{Set}$ where $F(X_1, X_2) = X_1 \times X_2$ for all sets X_1, X_2 and $F(f_1, f_2) = f_1 \times f_2$ for all functions $f_i: X_i \rightarrow Y_i$.

This functor fits nicely into our theory since it preserves pullbacks. Although the proof is simple and, of course, similar to the one for the input functor (Lemma 5.4.33) we provide it here.

Lemma 5.4.53 The product bifunctor preserves pullbacks.

Proof. If we have pullbacks in Set as indicated in the left of the diagram below ($i \in \{1, 2\}$), then we have to show that the right diagram is a pullback.

$$\begin{array}{ccc}
 P_i & \xrightarrow{a_i} & A_i \\
 b_i \downarrow & & \downarrow f_i \\
 B_i & \xrightarrow{g_i} & C_i
 \end{array}
 \qquad
 \begin{array}{ccc}
 P_1 \times P_2 & \xrightarrow{a_1 \times a_2} & A_1 \times A_2 \\
 b_1 \times b_2 \downarrow & & \downarrow f_1 \times f_2 \\
 B_1 \times B_2 & \xrightarrow{g_1 \times g_2} & C_1 \times C_2
 \end{array}$$

Commutativity of the right diagram is immediate by commutativity of the left diagrams because $(f_1 \times f_2) \circ (a_1 \times a_2) = (f_1 \circ a_1) \times (f_2 \circ a_2) = (g_1 \circ b_1) \times (g_2 \circ b_2) = (g_1 \times g_2) \circ (b_1 \times b_2)$. Moreover, for any set Q along with functions $a: Q \rightarrow A_1 \times A_2$, $b: Q \rightarrow B_1 \times B_2$ satisfying $(f_1 \times f_2) \circ a = (g_1 \times g_2) \circ b$ we take the projections $\pi_i: A_1 \times A_2 \rightarrow A_i$, $\tau_i: B_1 \times B_2 \rightarrow B_i$ and observe that we have $(f_1 \circ (\pi_1 \circ a)) \times (f_2 \circ (\pi_2 \circ a)) = (f_1 \times f_2) \circ a = (g_1 \times g_2) \circ b = (g_1 \circ (\tau_1 \circ b)) \times (g_2 \circ (\tau_2 \circ b))$. Thus there are unique functions $p_i: Q \rightarrow P_i$ such that $a_i \circ p_i = \pi_i \circ a$ and $b_i \circ p_i = \tau_i \circ b$ and we conclude that $(a_1 \times a_2) \circ \langle p_1, p_2 \rangle = a$ and $(b_1 \times b_2) \circ \langle p_1, p_2 \rangle = b$. Moreover, it is unique because for any function $\langle q_1, q_2 \rangle: Q \rightarrow P_1 \times P_2$ we must have $q_i = p_i$ by uniqueness of the p_i . \square

Let us now discuss possible evaluation functions for this functor. They are similar to the ones for the input functor in Example 5.4.34 but we add some additional parameters (this could be done analogously for the input functor).

Lemma 5.4.54 (Evaluation Functions for the Product Bifunctor) Let F be the product bifunctor. The evaluation functions $ev_F: [0, \top]^2 \rightarrow [0, \top]$ presented in the table below are well-behaved.

Maximal Distance \top	Other Parameters	$ev_F(r_1, r_2)$
$\top \in]0, \infty]$	$c_1, c_2 \in]0, 1]$	$\max\{c_1 r_1, c_2 r_2\}$
$\top = \infty$	$c_1, c_2 \in]0, \infty[, p \in \mathbb{N}$	$(c_1 x_1^p + c_2 x_2^p)^{1/p}$
$\top \in]0, \infty[$	$c_1, c_2 \in]0, 1], c_1 + c_2 \leq 1, p \in \mathbb{N}$	$(c_1 x_1^p + c_2 x_2^p)^{1/p}$

Proof. Apparently the only difference between the second and the third row is the range of the parameters. It ensures that $ev_F(r_1, r_2) \in [0, \top]$.

We proceed by checking all three conditions for well-behavedness:

W1. Let $f_i, g_i: X_i \rightarrow [0, \top]$ with $f_i \leq g_i$ be given. For the maximum we have

$$\tilde{F}(f_1, f_2) = \max\{c_1 f_1, c_2 f_2\} \leq \max\{c_1 g_1, c_2 g_2\} = \tilde{F}(g_1, g_2)$$

and for the second evaluation function, we also obtain

$$\begin{aligned} \tilde{F}(f_1, f_2) &= (c_1 \cdot f_1^p + c_2 \cdot f_2^p)^{1/p} \\ &\leq (c_1 \cdot g_1^p + c_2 \cdot g_2^p)^{1/p} = \tilde{F}(g_1, g_2) \end{aligned}$$

due to monotonicity of all involved functions since $c_1, c_2 > 0$.

W2. Let $\pi_i: [0, \top]^2 \rightarrow [0, \top]$ be the projections of the product and define $t := (x_{11}, x_{21}, x_{12}, x_{22}) \in F([0, \top]^2, [0, \top]^2) = [0, \top]^2 \times [0, \top]^2$. We have to show

the inequality

$$d_e(\tilde{F}(\pi_1, \pi_1)(t), \tilde{F}(\pi_2, \pi_2)(t)) \leq \tilde{F}(d_e, d_e)(t). \quad (5.4.10)$$

To do this, we first observe that the right hand side of this inequality evaluates to $\tilde{F}(d_e, d_e)(t) = \text{ev}_F(d_e(x_{11}, x_{21}), d_e(x_{12}, x_{22}))$. Moreover, we have $\tilde{F}(\pi_i, \pi_i)(t) = \text{ev}_F(x_{i1}, x_{i2})$ so if we define $z_i = \text{ev}_F(x_{i1}, x_{i2})$ the left hand side of (5.4.10) can be rewritten as $d_e(z_1, z_2)$. Thus (5.4.10) is equivalent to

$$d_e(z_1, z_2) \leq \text{ev}_F(d_e(x_{11}, x_{21}), d_e(x_{12}, x_{22})). \quad (5.4.11)$$

If $z_1 = z_2$ this is obviously true because $d_e(z_1, z_2) = 0$ and the right hand side of (5.4.11) is non-negative. We now assume $z_1 > z_2$ (the other case is symmetrical). For $\infty = z_1 > z_2$ inequality (5.4.11) holds because then $x_{11} = \infty$ or $x_{12} = \infty$ and $x_{21}, x_{22} < \infty$ (otherwise we would have $z_2 = \infty$) so both the left hand side and the right hand side are ∞ . Thus we can now restrict our attention to $\infty > z_1 > z_2$ where necessarily also $x_{11}, x_{12}, x_{21}, x_{22} < \infty$ (otherwise we would have $z_1 = \infty$ or $z_2 = \infty$). According to Lemma 5.2.2 (page 136), the inequality (5.4.11) is equivalent to showing the two inequalities

$$\begin{aligned} z_1 &\leq z_2 + \text{ev}_F(d_e(x_{11}, x_{21}), d_e(x_{12}, x_{22})), \quad \text{and} \\ z_2 &\leq z_1 + \text{ev}_F(d_e(x_{11}, x_{21}), d_e(x_{12}, x_{22})). \end{aligned}$$

By our assumption ($\infty > z_1 > z_2$) the second of these inequalities is satisfied, so we just have to show the first.

1. For the discounted maximum as evaluation function we have $z_i = \max\{c_1 x_{i1}, c_2 x_{i2}\}$. If for z_1 the maximum is attained for the first element, i.e., if $z_1 = c_1 x_{11}$, we can conclude that

$$\begin{aligned} z_2 + \max\{c_1 d_e(x_{11}, x_{21}), c_2 d_e(x_{12}, x_{22})\} &\geq z_2 + c_1 d_e(x_{11}, x_{21}) \\ &= z_2 + c_1 |x_{11} - x_{21}| \geq z_2 + c_1 (x_{11} - x_{21}) \\ &= z_2 + c_1 x_{11} - c_1 x_{21} = z_2 + z_1 - c_1 x_{21} \\ &= z_1 + (z_2 - c_1 x_{21}) \geq z_1 \end{aligned}$$

because $z_2 = \max\{c_1 x_{21}, c_2 x_{22}\} > c_1 x_{21}$ and therefore $(z_2 - c_1 x_{21}) \geq 0$. The same line of argument can be applied if $z_1 = c_2 x_{12}$.

2. For the second evaluation function we aim at using the Minkowski Inequality for Sums (Theorem 5.2.4, page 137) which tells us that

$$\left(|a_1|^p + |a_2|^p\right)^{1/p} + \left(|b_1|^p + |b_2|^p\right)^{1/p} \geq \left(|a_1 + b_1|^p + |a_2 + b_2|^p\right)^{1/p}$$

holds for all real numbers a_1, a_2, b_1, b_2 . Specifically, if we define the non-negative real numbers

$$a_1 := c_1^{1/p} x_{21}, \quad a_2 := c_2^{1/p} x_{22}$$

and the real numbers

$$b_1 := c_1^{1/p} \cdot (x_{11} - x_{21}), \quad b_2 := c_2^{1/p} \cdot (x_{12} - x_{22}).$$

we obtain the following parts:

$$\begin{aligned} \left(|a_1|^p + |a_2|^p\right)^{1/p} &= \left(c_1 x_{21}^p + c_2 x_{22}^p\right)^{1/p} = \text{ev}_F(x_{21}, x_{22}) = z_2 \\ \left(|b_1|^p + |b_2|^p\right)^{1/p} &= \left(c_1 |x_{11} - x_{21}|^p + c_2 |x_{12} - x_{22}|^p\right)^{1/p} \\ &= \left(c_1 d_e(x_{11}, x_{21})^p + c_2 d_e(x_{12}, x_{22})^p\right)^{1/p} \\ |a_1 + b_1|^p &= \left|c_1^{1/p} x_{21} + c_1^{1/p} \cdot (x_{11} - x_{21})\right|^p = c_1 |x_{11}|^p = c_1 x_{11}^p \\ |a_2 + b_2|^p &= \left|c_2^{1/p} x_{22} + c_2^{1/p} \cdot (x_{12} - x_{22})\right|^p = c_2 |x_{12}|^p = c_2 x_{12}^p \end{aligned}$$

and thus the Minkowski inequality yields

$$z_2 + \left(c_1 d_e(x_{11}, x_{21})^p + c_2 d_e(x_{12}, x_{22})^p\right)^{1/p} \geq \left(c_1 x_{11}^p + c_2 x_{12}^p\right)^{1/p} = z_1$$

which concludes the proof.

W₃. Both evaluation functions satisfy Condition W₃ of Definition 5.4.39, because we have

$$F(i, i)[F(\{0\}, \{0\})] = (i \times i)[\{0\} \times \{0\}] = \{(0, 0)\}$$

and for both evaluation functions apparently $\text{ev}_F^{-1}[\{0\}] = \{(0, 0)\}$. □

Using these well-behaved evaluation functions we can now lift the product bifunctor using our multifunctor lifting framework.

Lemma 5.4.55 (Product Pseudometrics) Let F be the product bifunctor of Definition 5.4.52. For the evaluation functions presented in Lemma 5.4.54 the Kantorovich-Rubinstein duality holds and the supremum [infimum] of the Kantorovich [Wasserstein] pseudometric is always a maximum [minimum]. Moreover, for all pseudometric spaces (X_1, d_1) , (X_2, d_2) we obtain the lifted pseudometrics $(d_1, d_2)^F: (X_1 \times X_2)^2 \rightarrow [0, \top]$ as given in the table below.

$\text{ev}_F(r_1, r_2)$	$(d_1, d_2)^F((x_1, x_2), (y_1, y_2))$
$\max\{c_1 r_1, c_2 r_2\}$	$\max\{c_1 d_1(x_1, y_1), c_2 d_2(x_2, y_2)\}$
$(c_1 x_1^p + c_2 x_2^p)^{1/p}$	$(c_1 d_1(x_1, y_1)^p + c_2 d_2(x_2, y_2)^p)^{1/p}$

Proof. We have already seen that the product bifunctor preserves weak pullbacks and that the given evaluation functions are well-behaved. We now first prove (for both evaluation functions) that the product functor satisfies the Kantorovich-Rubinstein duality and simultaneously that the supremum (in the Kantorovich pseudometric) is a maximum and the infimum (of the Wasserstein pseudometric) is a minimum.

Let $(X_1, d_1), (X_2, d_2)$ be pseudometric spaces, $\pi_i: X_i^2 \rightarrow X_i$ and $\tau_i: X_i^2 \rightarrow X_i$ be the projections and let $t_1 = (x_1, x_2), t_2 = (y_1, y_2) \in F(X_1, X_2) = X_1 \times X_2$ be given. We define $t := (x_1, y_1, x_2, y_2) \in F(X_1^2, X_2^2)$ and observe that $F(\pi_1, \tau_1)(t) = t_1$, $F(\pi_2, \tau_2)(t) = t_2$ and thus $t \in \Gamma_F(t_1, t_2)$ is a coupling of t_1 and t_2 . In the following we will construct nonexpansive functions $f_i: (X_i, d_i) \rightarrow ([0, \top], d_e)$ such that $d_e(\tilde{F}(f_1, f_2)(t_1), \tilde{F}(f_1, f_2)(t_2)) = \tilde{F}(d_1, d_2)(t)$ holds. Due to Theorem 5.4.51 (page 175) we can then conclude that duality holds and both supremum and infimum are attained.

1. For the first evaluation function in the table above we have $\tilde{F}(d_1, d_2)(t) = \max\{c_1 d_1(x_1, y_1), c_2 d_2(x_2, y_2)\}$ and assume without loss of generality that $c_1 d_1(x_1, y_1)$ is the maximal element. We define $f_1 := d_1(x_1, _)$, which is nonexpansive due to Lemma 5.2.9 (page 140), and f_2 to be the constant zero-function which is obviously nonexpansive as a constant function. Then we have:

$$\begin{aligned}
& d_e(\tilde{F}(f_1, f_2)(t_1), \tilde{F}(f_1, f_2)(t_2)) \\
&= d_e(\max\{c_1 f_1(x_1), c_2 f_2(x_2)\}, \max\{c_1 f_1(y_1), c_2 f_2(y_2)\}) \\
&= d_e(\max\{c_1 f_1(x_1), 0\}, \max\{c_1 f_1(y_1), 0\}) = d_e(c_1 f_1(x_1), c_1 f_1(y_1)) \\
&= c_1 d_1(x_1, y_1) = \max\{c_1 d_1(x_1, y_1), c_2 d_2(x_2, y_2)\} = \tilde{F}(d_1, d_2)(t)
\end{aligned}$$

The case where $c_2 d_2(x_2, y_2)$ is the maximal element is treated analogously.

2. For the second evaluation function we define $f_1 := d_1(x_1, _)$ and $f_2 := d_2(x_2, _)$ which are nonexpansive by Lemma 5.2.9 and obtain

$$\begin{aligned}
& d_e(\tilde{F}(f_1, f_2)(t_1), \tilde{F}(f_1, f_2)(t_2)) \\
&= d_e((c_1 f_1^p(x_1) + c_2 f_2^p(x_2))^{1/p}, (c_1 f_1^p(y_1) + c_2 f_2^p(y_2))^{1/p}) \\
&= d_e(0, (c_1 d_1^p(x_1, y_1) + c_2 d_2^p(x_2, y_2))^{1/p})
\end{aligned}$$

$$= (c_1 d_1^p(x_1, y_1) + c_2 d_2^p(x_2, y_2))^{1/p} = \tilde{F}(d_1, d_2)(t)$$

which completes the proof. \square

While all the product pseudometrics which we can obtain as lifting of the product functor by Lemma 5.4.55 are well-known, we point out a specifically interesting one, the undiscounted maximum pseudometric.

Lemma 5.4.56 (Binary Products in PMet) If we set $c_1 = c_2 = 1$ for the first evaluation function in Lemma 5.4.55 we obtain for two given pseudometric spaces (X_1, d_1) , (X_2, d_2) as lifted pseudometric the function $d_\infty: (X_1 \times X_2)^2 \rightarrow [0, \top]$, $d((x_1, x_2), (y_1, y_2)) = \max\{d_1(x_1, y_1), d_2(x_2, y_2)\}$. The resulting pseudometric space $(X_1 \times X_2, d_\infty)$ is exactly the categorical product of (X_1, d_1) and (X_2, d_2) in PMet.

Proof. This follows immediately from Theorem 5.2.8 (page 138) by taking $I = 2$ as index category, and $f_i = \pi_i: X_1 \times X_2 \rightarrow X$. \square

In a completely analogous way as for the product bifunctor, we will now introduce and study the coproduct bifunctor.

Definition 5.4.57 (Coproduct Bifunctor) The *coproduct bifunctor* is the functor $F: \text{Set}^2 \rightarrow \text{Set}$, where $F(X_1, X_2) = X_1 + X_2$ for all sets X_1, X_2 and $F(f_1, f_2) = f_1 + f_2$ for all functions $f_1: X_1 \rightarrow Y_1$, $f_2: X_2 \rightarrow Y_2$. Explicitly¹², the function $f_1 + f_2: X_1 + X_2 \rightarrow Y_1 + Y_2$ is given via the assignment $f_1 + f_2(x, i) = (f_i(x), i)$.

As for the product bifunctor, we can show that this bifunctor preserves pullbacks.

Lemma 5.4.58 The coproduct bifunctor preserves pullbacks.

Proof. If we have pullbacks in Set as indicated in the left of the diagram below ($i \in \{1, 2\}$), then we have to show that the right diagram is a pullback.

$$\begin{array}{ccc} P_i & \xrightarrow{a_i} & A_i \\ b_i \downarrow & & \downarrow f_i \\ B_i & \xrightarrow{g_i} & C_i \end{array} \qquad \begin{array}{ccc} P_1 + P_2 & \xrightarrow{a_1 + a_2} & A_1 + A_2 \\ b_1 + b_2 \downarrow & & \downarrow f_1 + f_2 \\ B_1 + B_2 & \xrightarrow{g_1 + g_2} & C_1 + C_2 \end{array}$$

¹²Remember that $X_1 + X_2 \cong X_1 \times \{1\} \cup X_2 \times \{2\}$.

Commutativity of the right diagram is immediate by commutativity of the left diagrams because for any $(x, i) \in P_1 + P_2$ we have $(f_1 + f_2) \circ (a_1 + a_2)(x, i) = f_i \circ a_i(x) = g_i \circ b_i(x) = (g_1 + g_2) \circ (b_1 + b_2)(x, i)$. Moreover, for any set Q along with functions $a: Q \rightarrow A_1 + A_2$, $b: Q \rightarrow B_1 + B_2$ satisfying $(f_1 + f_2) \circ a = (g_1 + g_2) \circ b$ we define the sets $Q_i := \{x \in Q \mid \exists y \in Y. a(x) = (y, i)\} = \{x \in Q \mid \exists y \in Y. b(x) = (y, i)\}$ and observe that we obtain a disjoint partition of Q , i.e., $Q_1 \cap Q_2 = \emptyset$ and $Q = Q_1 \cup Q_2$. Additionally, we have $f_i \circ a|_{Q_i} = g_i \circ b|_{Q_i}$ so there are unique functions $p_i: Q_i \rightarrow P_i$ such that $a_i \circ p_i = a|_{Q_i}$ and $b_i \circ p_i = b|_{Q_i}$. We define the function

$$p: Q \rightarrow P_1 + P_2, \quad p(x) = \begin{cases} p_1(x), & \text{if } x \in Q_1 \\ p_2(x), & \text{if } x \in Q_2 \end{cases}$$

and conclude that $(a_1 + a_2) \circ p = a$ and $(b_1 + b_2) \circ p = b$. Moreover, it is unique because for any function $q: Q \rightarrow P_1 \times P_2$ we must have $q|_{Q_i} = p_i$ by uniqueness of the p_i . \square

For this functor we will just consider one type of evaluation function whose only parameter is the maximal element \top .

Lemma 5.4.59 (Evaluation Function for the Coproduct Bifunctor) Let F be the coproduct bifunctor. The evaluation function $ev_F: [0, \top] + [0, \top] \rightarrow [0, \top]$, where $ev_F(x, i) = x$, is well-behaved.

Proof. We show the three properties of a well-behaved evaluation function.

W1. Let $f_1, f_2, g_1, g_2: X \rightarrow [0, \top]$ with $f_1 \leq g_1$, $f_2 \leq g_2$ and $(z, i) \in F(X_1, X_2) = X_1 + X_2$. We have

$$\begin{aligned} \tilde{F}(f_1, f_2)(z, i) &= ev_F(F(f_1, f_2)(z, i)) \\ &= f_i(z) \leq g_i(z) = ev_F(F(g_1, g_2)(z, i)) = \tilde{F}(g_1, g_2)(z, i). \end{aligned}$$

W2. Let $t = ((x, y), i) \in F([0, \top]^2, [0, \top]^2) = [0, \top]^2 \times \{1, 2\}$. We obtain equality:

$$\begin{aligned} \tilde{F}(d_e, d_e)(t) &= ev_F(d_e(x, y), i) = d_e(x, y) \\ &= d_e(ev_F(x, i), ev_F(y, i)) = d_e(\tilde{F}(\pi_1, \pi_1)(t), \tilde{F}(\pi_2, \pi_2)(t)). \end{aligned}$$

W3. Let $i: 0 \hookrightarrow [0, \top]$ be the inclusion function. We have $Fi[F(\{0\}, \{0\})] = (i + i)[\{0\} + \{0\}] = \{0\} \times \{1, 2\} = ev_F^{-1}[\{0\}]$. \square

With this evaluation function we can now employ our multifunctor lifting framework to obtain the following coproduct pseudometric.

Lemma 5.4.60 (Coproduct Pseudometric) For the coproduct bifunctor of Definition 5.4.57 and the evaluation function of Lemma 5.4.59 the Kantorovich-Rubinstein duality holds, the supremum of the Kantorovich pseudometric is always a maximum, the infimum of the Wasserstein pseudometric is a minimum whenever a coupling exists and we obtain the coproduct pseudometric

$$d_+ : (X_1 + X_2)^2 \rightarrow [0, \top], \quad d_+((x_1, i_1), (x_2, i_2)) = \begin{cases} d_i(x_1, x_2), & \text{if } i_1 = i_2 = i \\ \top, & \text{else} \end{cases}.$$

Proof. We already know that the coproduct functor preserves weak pullbacks and that the evaluation function is well-behaved. Now we show that the pair of functor and evaluation function ev_F satisfies the Kantorovich-Rubinstein duality and simultaneously that the supremum (in the Kantorovich pseudometric) is a maximum and the infimum (of the Wasserstein pseudometric) is a minimum if and only if there exists a coupling of the two given elements.

Let $(X_1, d_1), (X_2, d_2)$ be pseudometric spaces, $\pi_i : X_1^2 \rightarrow X_1$ and $\tau_i : X_2^2 \rightarrow X_2$ be the projections and $t_1, t_2 \in F(X_1, X_2) = X_1 + X_2$, say $t_1 = (z, i)$, $t_2 = (z', i')$. We distinguish two cases.

1. For $i = i'$ we define $t = ((z, z'), i)$ and observe that $F(\pi_1, \tau_1)((z, z'), i) = t_1$, $F(\pi_2, \tau_2)((z, z'), i) = t_2$, thus $t \in \Gamma_F(t_1, t_2)$. Furthermore $\tilde{F}(d_1, d_2)(t) = d_i(z, z')$. If $i = i' = 1$ we define $f_1 := d_1(z, _): (X_1, d_1) \rightarrow ([0, \top], d_e)$ which is nonexpansive according to Lemma 5.2.9 and consider an arbitrary nonexpansive function $f_2 : (X_2, d_2) \rightarrow ([0, \top], d_e)$ (e.g. the constant zero-function). Then we have:

$$\begin{aligned} d_e(\tilde{F}(f_1, f_2)(t_1), \tilde{F}(f_1, f_2)(t_2)) &= d_e(\tilde{F}(f_1, f_2)(z, 1), \tilde{F}(f_1, f_2)(z', 1)) \\ &= d_e(f_1(z), f_1(z')) = d_e(0, d_1(z, z')) \\ &= d_1(z, z') = d_i(z, z'). \end{aligned}$$

The case $i = i' = 2$ can be treated analogously.

2. In the case where $i \neq i'$, there is no coupling that projects to (z, i) and (z', i') , thus $(d_1, d_2)^{\downarrow F}(t_1, t_2) = \top$. We show that also $(d_1, d_2)^{\uparrow F}(t_1, t_2) = \top$. We define f_1 to be the constant 0-function and f_2 the constant \top -function. We have:

$$\begin{aligned} d_e(\tilde{F}(f_1, f_2)(t_1), \tilde{F}(f_1, f_2)(t_2)) &= d_e(\tilde{F}(f_1, f_2)(z, i), \tilde{F}(f_1, f_2)(z', j)) \\ &= d_e(f_i(z), f_j(z')) = d_e(0, \top) = \top \end{aligned}$$

which completes the proof. □

We conclude this section by the observation that – as before – this yields the categorical coproduct.

Lemma 5.4.61 (Binary Coproducts in PMet) The pseudometric space $(X_1 + X_2, d_+)$ where d_+ is the pseudometric given in Lemma 5.4.60 is exactly the categorical coproduct of (X_1, d_1) and (X_2, d_2) in PMet.

Proof. This follows immediately from Theorem 5.2.8 by taking $I = 2$ as index category, and $f_i = \iota_i: X_i \rightarrow X_1 + X_2$. \square

5.5 Bisimilarity Pseudometrics

In this section we now want to use our lifting framework to derive bisimilarity pseudometrics. We assume an arbitrary lifting $\bar{F}: \text{PMet} \rightarrow \text{PMet}$ of an endofunctor F on Set and, for any pseudometric space (X, d) , we write d^F for the pseudometric obtained by applying \bar{F} to (X, d) . Such a lifting can be obtained as an endofunctor lifting, by taking a lifted multifunctor and fixing all parameters apart from one as in Lemma 5.4.37, or by the composition of such functors.

Our first result ensures that if $z: Z \rightarrow FZ$ is a final F -coalgebra, then there is also a final \bar{F} -coalgebra which is constructed by simply enriching Z with a suitable pseudometric d_Z .

Theorem 5.5.1 (Final Coalgebra Construction for Liftings) Let the functor $\bar{F}: \text{PMet} \rightarrow \text{PMet}$ be a lifting of a functor $F: \text{Set} \rightarrow \text{Set}$. We require that F has a final coalgebra $z: Z \rightarrow FZ$. For every ordinal i we construct a pseudometric $d_i: Z \times Z \rightarrow [0, \top]$ as follows:

- ▷ $d_0 := 0$ is the zero pseudometric,
- ▷ $d_{i+1} := d_i^F \circ (z \times z)$ for all ordinals i and
- ▷ $d_j = \sup_{i < j} d_i$ for all limit ordinals j .

This sequence converges for some ordinal θ , i.e, we reach a fixed point $d_\theta = d_\theta^F \circ (z \times z)$. Moreover, the resulting isomorphism $z: (Z, d_\theta) \rightarrow (FZ, d_\theta^F)$ is the final \bar{F} -coalgebra.

Proof. It can be easily shown that each of the d_i is a pseudometric, since the supremum of pseudometrics is again a pseudometric. Since d_θ is a fixed-point, z is an isometry and hence nonexpansive. Furthermore the chain converges once we reach an ordinal whose cardinality is larger than the cardinality of the lattice of pseudometrics on Z . We now proceed to show that we obtain the final coalgebra for \bar{F} .

Let $c: (X, d) \rightarrow \bar{F}(X, d)$ be any \bar{F} -coalgebra. Obviously there is an underlying F -coalgebra $c: X \rightarrow FX$ in Set . Since z is the final F -coalgebra, there exists a unique function $f: X \rightarrow Z$ such that $z \circ f = Ff \circ c$. It is left to show that f is a nonexpansive function $(X, d) \rightarrow (Z, d_\theta)$.

For each ordinal i we define a pseudometric $e_i: X \times X \rightarrow [0, \top]$ as follows:

- ▷ e_0 is the constant zero-pseudometric,
- ▷ $e_{i+1} := e_i^F \circ (c \times c)$ and
- ▷ $e_j := \sup_{i < j} e_i$ if j is a limit ordinal.

We show that $e_i \leq d$: Obviously $e_0 \leq d$ and furthermore $e_{i+1} = e_i^F \circ (c \times c) \leq d^F \circ (c \times c) \leq d$ where the first inequality is due to the fact that the lifting preserves the order on pseudometrics (see Theorem 5.4.2, page 144) and the second is nonexpansiveness of c . If we take the limit $e_j = \sup_{i < j} e_i$, we know that $e_i \leq d$ for each $i < j$ and hence also $e_j \leq d$.

As an auxiliary step we will prove that all $f: (X, e_i) \rightarrow (Z, d_i)$ are nonexpansive. This holds for $i = 0$ since for all $x, y \in X$ we have $e_0(x, y) = 0 = d_0(f(x), f(y))$. For $i + 1$ we have

$$\begin{aligned} d_{i+1}(f(x), f(y)) &= d_i^F \circ (z \times z)(f(x), f(y)) = d_i^F((z \circ f)(x), (z \circ f)(y)) \\ &= d_i^F((Ff \circ c)(x), (Ff \circ c)(y)) = d_i^F(Ff(c(x)), Ff(c(y))) \\ &\leq e_i^F(c(x), c(y)) = e_{i+1}(x, y). \end{aligned}$$

The inequality above holds since if $f: (X, e_i) \rightarrow (Z, d_i)$ is a nonexpansive function also $\bar{F}f: (FX, e_i^F) \rightarrow (FZ, d_i^F)$ is nonexpansive. Whenever j is a limit ordinal we obtain:

$$d_j(f(x), f(y)) = \sup_{i < j} d_i(f(x), f(y)) \leq \sup_{i < j} e_i(x, y) = e_j(x, y).$$

Finally, we combine this result with the result from above ($e_i \leq d$ for all ordinals i) to obtain the inequality $d_\theta(f(x), f(y)) \leq e_\theta(x, y) \leq d(x, y)$ which shows that $f: (X, d) \rightarrow (Z, d)$ is nonexpansive. Thus, if we equip Z with d_θ it is indeed the final \bar{F} -coalgebra. \square

We remark that the above construction apparently defines d_θ as least fixed point (with regard to the pointwise order of pseudometrics) of the equation

$$d_\theta = d^F \circ (z \times z).$$

As a first simple example of this construction we consider the machine functor. We will look at more examples at the end of this section.

Example 5.5.2 (Final Coalgebra for the Lifted Machine Functor) We consider the machine endofunctor $M_2 = 2 \times _^A$. As maximal distance we take $\top = 1$ and as evaluation function we use $ev_{M_2}: [0, 1] \times [0, 1]^A \rightarrow [0, 1]$ with $ev_{M_2}(o, s) = c \cdot \max_{a \in A} s(a)$ for $0 < c < 1$ as in Example 5.4.35 (page 169).

We recall from Example 2.4.10 (page 54) that the carrier of the final M_2 -coalgebra is 2^{A^*} . Moreover, from Example 5.4.35 we know that for any pseudometric d on 2^{A^*} we obtain as Wasserstein pseudometric the function $d^{\downarrow F}: (2 \times (2^{A^*})^A)^2 \rightarrow [0, 1]$ where, for all $(o_1, s_1), (o_2, s_2) \in 2 \times (2^{A^*})^A$,

$$d^{\downarrow F}((o_1, s_1), (o_2, s_2)) = \max \left\{ d_2(o_1, o_2), c \cdot \max_{a \in A} d(s_1(a), s_2(a)) \right\}$$

with the discrete metric d_2 on 2 . Thus the fixed-point equation induced by Theorem 5.5.1 is given by, for $L_1, L_2 \in 2^{A^*}$,

$$d(L_1, L_2) = \max \left\{ d_2(L_1(\varepsilon), L_2(\varepsilon)), c \cdot \max_{a \in A} d(\lambda w. L_1(aw), \lambda w. L_2(aw)) \right\}.$$

Now because d_2 is the discrete metric with $d_2(0, 1) = 1$ we can easily see that $d_{2^{A^*}}$ as defined below is indeed the least fixed-point of this equation and thus $(2^{A^*}, d_{2^{A^*}})$ is the carrier of the final \overline{M}_2 -coalgebra.

$$d_{2^{A^*}}: 2^{A^*} \times 2^{A^*} \rightarrow [0, 1], \quad d_{2^{A^*}}(L_1, L_2) = c^{\inf\{n \in \mathbb{N} \mid \exists w \in A^n. L_1(w) \neq L_2(w)\}}.$$

Thus the distance between two languages $L_1, L_2: A^* \rightarrow 2$ can be determined by looking for a word w of minimal length which is contained in one and not in the other. Then, the distance is computed as $c^{|w|}$. This is similar to a standard ultrametric between traces [BN80].

We already noted in the beginning of this chapter that for any set X , the set of pseudometrics over X , with pointwise order, is a complete lattice. Moreover, by Theorem 5.4.2 the lifting $\bar{_}$ induces a monotone function $_^F$ which maps any pseudometric d on X to d^F on FX . If, additionally, such function is ω -continuous, i.e., if it preserves the supremum of ω -chains, the construction in Theorem 5.5.1 will apparently converge in at most ω steps, i.e., $d_0 = d_\omega$. It is easy to see that this is the case in Example 5.5.2 and we show below¹³ that the liftings induced by the finite powerset functor and the probability distribution functor with finite support are ω -continuous.

Theorem 5.5.3 (ω -continuity of the liftings of \mathcal{P}_f and \mathcal{D}_f) Let F be the finite powerset functor \mathcal{P}_f of Example 2.3.11 or the distribution functor \mathcal{D}_f (with

¹³Theorem 5.5.3 and its proof were developed entirely by Paolo Baldan. It was published in the extended version of our first paper on behavioral metrics [BBKK14, Proposition P.6.1].

finite support) of Example 2.3.12. For any set X the function $_^F$ mapping a pseudometric d on X to the pseudometric¹⁴ $d^F = d^{\uparrow F} = d^{\downarrow F}$ on FX is ω -continuous, i.e., for any increasing chain of pseudometrics $(d_i)_{i \in \mathbb{N}}$ on X , we have $(\sup_i d_i)^F = \sup_i d_i^F$.

Proof. Let X be a fixed set. By Theorem 5.4.2 (page 144), we know that for any lifting, the function $_^F$ is monotone, i.e., whenever $d_1 \leq d_2$ it holds that $d_1^F \leq d_2^F$.

Given an increasing chain of pseudometrics $(d_i)_{i \in \mathbb{N}}$ over X , simply by monotonicity of $_^F$ we can deduce that $\sup_i d_i^F \leq (\sup_i d_i)^F$ because for any $i \in \mathbb{N}$ we apparently have $d_i \leq \sup_i d_i$.

We next prove that for the Wasserstein/Kantorovich liftings of either \mathcal{P}_f or \mathcal{D}_f also the converse inequality holds. We proceed separately for the two functors.

1. *Finite powerset:* Let $d := \sup_i d_i$. We have to show $d^{\mathcal{P}_f} \leq \sup_i d_i^{\mathcal{P}_f}$. Let $X_1, X_2 \in \mathcal{P}_f(X)$ be finite subsets of X . Since X_1 and X_2 are finite and $d = \sup_i d_i$, for any $\varepsilon > 0$ we can find an $i \in \mathbb{N}$ such that for any $x_1 \in X_1, x_2 \in X_2$ and all $j \geq i$ we have $d(x_1, x_2) - d_j(x_1, x_2) \leq \varepsilon$. According to the definition of the Wasserstein lifting for \mathcal{P}_f we get for all $j \geq i$:

$$\begin{aligned} d^{\downarrow \mathcal{P}_f}(X_1, X_2) &= \inf \left\{ \max_{(x_1, x_2) \in W} d(x_1, x_2) \mid W \in \Gamma_{\mathcal{P}_f}(X_1, X_2) \right\} \\ &\leq \inf \left\{ \max_{(x_1, x_2) \in W} (d_j(x_1, x_2) + \varepsilon) \mid W \in \Gamma_{\mathcal{P}_f}(X_1, X_2) \right\} \\ &= \inf \left\{ \max_{(x_1, x_2) \in W} d_j(x_1, x_2) \mid W \in \Gamma_{\mathcal{P}_f}(X_1, X_2) \right\} + \varepsilon = d_j^{\downarrow \mathcal{P}_f}(X_1, X_2) + \varepsilon \end{aligned}$$

Therefore, $d^{\mathcal{P}_f}(X_1, X_2) \leq \sup_i d_i^{\mathcal{P}_f}(X_1, X_2) + \varepsilon$. Given that ε can be arbitrarily small, we deduce that indeed $d^{\mathcal{P}_f}(X_1, X_2) \leq \sup_i d_i^{\mathcal{P}_f}(X_1, X_2)$, as desired.

2. *Finitely supported distributions.* Let us denote $d = \sup_i d_i$. We have to show $d^{\mathcal{D}_f} \leq \sup_i d_i^{\mathcal{D}_f}$. Let $P_1, P_2 \in \mathcal{D}_f X$ and let X_1, X_2 be the corresponding finite supports of P_1 and P_2 , namely $X_i = \{x \in X \mid P_i(x) > 0\}$. As before, since X_1 and X_2 are finite and $d = \sup_i d_i$, for any $\varepsilon > 0$ we can find an $i \in \mathbb{N}$ such that for any $x_1 \in X_1, x_2 \in X_2$ and $j \geq i$ we have $d(x_1, x_2) - d_j(x_1, x_2) \leq \varepsilon$. Using the definition of the Wasserstein lifting for the functor \mathcal{D}_f , we get for all $j \geq i$:

$$d^{\downarrow \mathcal{D}_f}(X_1, X_2) = \inf \left\{ \sum_{x_1, x_2 \in X} d(x_1, x_2) \cdot P(x_1, x_2) \mid P \in \Gamma_{\mathcal{D}_f}(P_1, P_2) \right\}$$

¹⁴Recall that by Examples 5.4.30 and 5.4.31 the duality holds for both functors, i.e., the Wasserstein and Kantorovich lifting coincide.

since for any $(x_1, x_2) \in X \times X$, if $(x_1, x_2) \notin X_1 \times X_2$ necessarily $P(x_1, x_2) = 0$

$$\begin{aligned}
&= \inf \left\{ \sum_{(x_1, x_2) \in X_1 \times X_2} d(x_1, x_2) \cdot P(x_1, x_2) \mid P \in \Gamma_{\mathcal{D}_f}(P_1, P_2) \right\} \\
&\leq \inf \left\{ \sum_{(x_1, x_2) \in X_1 \times X_2} (d_j(x_1, x_2) + \varepsilon) \cdot P(x_1, x_2) \mid P \in \Gamma_{\mathcal{D}_f}(P_1, P_2) \right\} \\
&= \inf \left\{ \sum_{(x_1, x_2) \in X_1 \times X_2} d_j(x_1, x_2) \cdot P(x_1, x_2) + \varepsilon \cdot \sum_{x_1, x_2 \in X} P(x_1, x_2) \mid P \in \Gamma_{\mathcal{D}_f}(P_1, P_2) \right\} \\
&= \inf \left\{ \sum_{(x_1, x_2) \in X_1 \times X_2} d_j(x_1, x_2) \cdot P(x_1, x_2) + \varepsilon \mid P \in \Gamma_{\mathcal{D}_f}(P_1, P_2) \right\} \\
&= \inf \left\{ \sum_{(x_1, x_2) \in X_1 \times X_2} d_j(x_1, x_2) \cdot P(x_1, x_2) \mid P \in \Gamma_{\mathcal{D}_f}(P_1, P_2) \right\} + \varepsilon \\
&= \inf \left\{ \sum_{x_1, x_2 \in X} d_j(x_1, x_2) \cdot P(x_1, x_2) \mid P \in \Gamma_{\mathcal{D}_f}(P_1, P_2) \right\} + \varepsilon = d_j^{\downarrow \mathcal{D}_f}(X_1, X_2) + \varepsilon
\end{aligned}$$

Therefore, $d^{\mathcal{D}_f}(X_1, X_2) \leq \sup_i d_i^{\mathcal{D}_f}(X_1, X_2) + \varepsilon$. Given that ε can be arbitrarily small, we deduce that indeed $d^{\mathcal{D}_f}(X_1, X_2) \leq \sup_i d_i^{\mathcal{D}_f}(X_1, X_2)$, as desired. \square

The lifting of the final F -coalgebra to a final \bar{F} -coalgebra, which is provided by Theorem 5.5.1, allows us to move from a qualitative to a qualitative behavior analysis: Instead of just considering equivalences, in PMet we can now measure the distance of behaviors using the final coalgebra.

Definition 5.5.4 (Bisimilarity Pseudometric) Let $\bar{F}: \text{PMet} \rightarrow \text{PMet}$ be a lifting of a Set -endofunctor F for which a final coalgebra exists. Moreover, let θ be the ordinal for which the final coalgebra construction of Theorem 5.5.1 converges. For any F -coalgebra $c: X \rightarrow FX$ the *bisimilarity distance* on X is the function $\text{bd}_c: X \times X \rightarrow [0, \top]$ where

$$\text{bd}_c(x, y) := d_\theta(\llbracket x \rrbracket_c, \llbracket y \rrbracket_c)$$

for all $x, y \in X$. Since d_θ is a pseudometric also bd_c is a pseudometric.

Let us check how this definition applies to deterministic automata and the machine bifunctor.

Example 5.5.5 (Bisimilarity Pseudometric for Deterministic Automata) We instantiate the above definition for the machine functor $M_2 = 2 \times _^A$ with maximal distance $\top = 1$ and evaluation function $ev_{M_2}: [0, 1] \times [0, 1]^A$ with $ev_{M_2}(0, s) = c \cdot \max_{a \in A} s(a)$ for $0 < c < 1$ as in Example 5.5.2. We recall from Example 2.4.10 (page 54) that for any coalgebra $\alpha: X \rightarrow 2 \times X^A$ the unique map $\llbracket \cdot \rrbracket_\alpha: X \rightarrow 2^{A^*}$ into the final coalgebra maps each state $x \in X$ to the (finite) language $\llbracket x \rrbracket_\alpha: A^* \rightarrow 2$ it accepts. Using the final coalgebra pseudometric from Example 5.5.2 we have

$$bd_\alpha: X \times X \rightarrow [0, 1], \quad bd_\alpha(x, y) = c^{\inf\{n \in \mathbb{N} \mid \exists w \in A^n. \llbracket x \rrbracket_\alpha(w) \neq \llbracket y \rrbracket_\alpha(w)\}}.$$

Thus the distance between two states $x, y \in X$ is determined by the shortest word w which is contained in the language of one state and not in the language of the other. Then the distance is computed as $c^{|w|}$.

We call the above pseudometric the *bisimilarity* pseudometric because states which are F-bisimilar in the sense of Definition 2.4.12 (page 56) have distance 0.

Theorem 5.5.6 Let $\bar{F}, F, \theta, c: X \rightarrow FX$ be as in Definition 5.5.4. For all $x, x' \in X$,

$$x \sim_c x' \implies bd_c(x, x') = 0.$$

Proof. By Theorem 2.4.14 (page 57) $x \sim_c x'$ implies $\llbracket x \rrbracket_c = \llbracket x' \rrbracket_c$. Moreover, since d_θ is a pseudometric it is reflexive and thus $bd_c(x, x') = d_\theta(\llbracket x \rrbracket_c, \llbracket y \rrbracket_c) = 0$. \square

We will later (Theorem 5.5.10, page 190) provide some sufficient conditions which guarantee that also the converse of the above implication holds.

Before doing so, we show that under some mild conditions the bisimilarity pseudometric can be computed analogously to d_θ itself, replacing the final coalgebra $z: Z \rightarrow FZ$ by the coalgebra $c: X \rightarrow FX$ under consideration. This way we do not have to explore the entire final coalgebra (which might be too large) but can restrict to the relevant part.

Theorem 5.5.7 (Bisimilarity Pseudometric Construction) Let the chain of the d_i converge in θ steps and \bar{F} preserve isometries. Let furthermore $c: X \rightarrow FX$ be an arbitrary coalgebra. For all ordinals i we define a pseudometric $e_i: X \times X \rightarrow [0, \top]$ as follows:

- ▷ e_0 is the zero pseudometric,
- ▷ $e_{i+1} = e_i^F \circ (c \times c)$ for all ordinals i and
- ▷ $e_j = \sup_{i < j} e_i$ for all limit ordinals j .

Then we reach a fixed point after $\zeta \leq \theta$ steps, i.e., $e_\zeta = e_\zeta^F \circ (c \times c)$. Moreover e_ζ is the bisimilarity pseudometric, i.e., we have $bd_c = e_\zeta$.

Proof. The chain e_i of metrics is the same as the one constructed in the proof of Theorem 5.5.1. In that proof we have shown that the unique coalgebra homomorphisms $f: X \rightarrow Z$ into the final coalgebra in \mathbf{Set} are nonexpansive when seen as functions $f: (X, e_i) \rightarrow (Z, d_i)$. Here we show that they are all in fact isometries.

- ▷ For $i = 0$ this is true: for $x, y \in X$ we have $d_0(f(x), f(y)) = 0 = e_0(x, y)$.
- ▷ Now assume that $f: (X, e_i) \rightarrow (Z, d_i)$ is an isometry, which implies (since \bar{F} preserves isometries) that $\bar{F}f: (FX, e_i^F) \rightarrow (FZ, d_i^F)$ is an isometry. Moreover, $z \circ f = Ff \circ c$ holds because f is a coalgebra homomorphism from c to z . Hence for $x, y \in X$ we have

$$\begin{aligned} d_{i+1}(f(x), f(y)) &= d_i^F(z(f(x)), z(f(y))) = d_i^F(Ff(c(x)), Ff(c(y))) \\ &= e_i^F(c(x), c(y)) = e_{i+1}(x, y). \end{aligned}$$

- ▷ For a limit ordinal j we have

$$d_j(f(x), f(y)) = \sup_{i < j} d_i(f(x), f(y)) = \sup_{i < j} e_i(x, y) = e_j(x, y).$$

We know that d_θ is a fixed-point, i.e., we have $d_\theta = d_\theta^F \circ (z \times z)$. Then e_θ must also be a fixed-point ($e_\theta = e_\theta^F \circ (c \times c)$), since:

$$\begin{aligned} e_\theta(x, y) &= d_\theta(f(x), f(y)) = d_\theta^F(z(f(x)), z(f(y))) = d_\theta^F(Ff(c(x)), Ff(c(y))) \\ &= e_\theta^F(c(x), c(y)) \end{aligned}$$

using again the fact that Ff is an isometry. Hence $\zeta \leq \theta$, i.e., the chain e_i might converge earlier and $bd_c(x, y) = d_\theta(f(x), f(y)) = e_\theta(x, y) = e_\zeta(x, y)$. \square

Let us now try to find conditions which ensure that two states x and y are bisimilar if their bisimilarity distance is 0. To this aim, we proceed by recalling the final coalgebra construction via the final chain which was first presented in the dual setting (free/initial algebra).

Definition 5.5.8 (Final Chain Construction [Ada74]) Let \mathfrak{C} be a category with terminal object $\mathbb{1}$ and limits of ordinal-indexed cochains. For any functor $F: \mathfrak{C} \rightarrow \mathfrak{C}$ the *final chain* consists of objects W_i for all ordinals i and *connection morphisms* $p_{i,j}: W_j \rightarrow W_i$ for all ordinals $i \leq j$. The objects are defined as

- ▷ $W_0 := \mathbb{1}$,
- ▷ $W_{i+1} := FW_i$ for all ordinals i , and
- ▷ $W_j := \lim_{i < j} W_i$ for all limit ordinals j .

The morphisms are determined by $p_{0,i} := !_{W_i}: W_i \rightarrow \mathbb{1}$, $p_{i,i} = \text{id}_{W_i}$ for all ordinals i , $p_{i+1,j+1} := Fp_{i,j}$ for all ordinals $i < j$ and if j is a limit ordinal the $p_{i,j}$ are the morphisms of the limit cone. They satisfy $p_{i,k} = p_{i,j} \circ p_{j,k}$ for all ordinals $i \leq j \leq k$. We say that the chain *converges* in λ steps if $p_{\lambda,\lambda+1}: W_{\lambda+1} \rightarrow W_\lambda$ is an isomorphism.

This construction does not necessarily converge (e.g. for the unrestricted powerset functor \mathcal{P} on Set), but if it does, we always obtain a final coalgebra.

Theorem 5.5.9 (Final Coalgebra via the Final Chain [Ada74]) Let \mathcal{C} be a category with terminal object $\mathbb{1}$ and limits of ordinal-indexed cochains. If the final chain of a functor $F: \mathcal{C} \rightarrow \mathcal{C}$ converges in λ steps then $p_{\lambda,\lambda+1}^{-1}: W_\lambda \rightarrow FW_\lambda$ is the final coalgebra.

We now show under which circumstances d_θ is a metric and how our construction relates to the construction of the final chain.

Theorem 5.5.10 (Final Coalgebra Metric) Let $\bar{F}: \text{PMet} \rightarrow \text{PMet}$ be a lifting of a functor $F: \text{Set} \rightarrow \text{Set}$ which has a final coalgebra $z: Z \rightarrow FZ$. Let θ be the ordinal for which the construction of the d_i in Theorem 5.5.1 converges. If

1. \bar{F} preserves isometries,
2. \bar{F} preserves metrics, and
3. the final chain for F converges

then d_θ is a metric, i.e., all for $z, z' \in Z$ we have $d_\theta(z, z') = 0 \iff z = z'$.

Proof. Let $W_i, p_{i,j}: W_j \rightarrow W_i$ be as in Definition 5.5.8. We construct a series of metrics $e_i: W_i \times W_i \rightarrow [0, \top]$ as follows:

- ▷ $e_0: \mathbb{1} \times \mathbb{1} \rightarrow [0, \top]$ is the (unique!) zero metric on $\mathbb{1}$,
- ▷ $e_{i+1} := e_i^F: W_{i+1} \times W_{i+1} \rightarrow [0, \top]$ for all ordinals i and
- ▷ $e_j := \sup_{i < j} e_i \circ (p_{i,j} \times p_{i,j})$ for all limit ordinals j .

Since the functor preserves metrics e_{i+1} is a metric if e_i is. Given a limit ordinal j we can easily check that e_j is a pseudometric provided that all the e_i with $i < j$ are pseudometrics. To see that e_j is also a metric when all e_i with $i < j$ are metrics we proceed as follows: Suppose $e_j(x, y) = 0$ for some $x, y \in W_j$,

then we know that for all $i < j$ we must have $e_i(p_{i,j}(x), p_{i,j}(y)) = 0$ and thus $p_{i,j}(x) = p_{i,j}(y)$ because the e_i are metrics. Since the cone $(W_j \xrightarrow{p_{i,j}} W_i)_{i < j}$ is by definition a limit in Set we can now conclude that $x = y$. This is due to the universal property of the limit: Let us assume $x \neq y$ then for the cone $(\{x, y\} \xrightarrow{f_i} W_i)_{i < j}$ with $f_i(x) := p_{i,j}(x)$, and also $f_i(y) := p_{i,j}(y) = p_{i,j}(y)$ there would have to be a unique function $u: \{x, y\} \rightarrow W_j$ satisfying $p_{i,j} \circ u = f_i$. However, for example $u, u': \{x, y\} \rightarrow W_j$ where $u(x) = u(y) = x$ and $u'(x) = u'(y) = y$ are distinct functions satisfying this commutativity which is a contradiction to the uniqueness. Thus our assumption $(x \neq y)$ is false and e_j is indeed a metric.

Using the metrics e_i we now consider the connection morphisms $p^i := p_{i,\lambda}: Z \rightarrow W_i$ and proceed by showing that each of these connection morphisms p_i is an isometry $(Z, d_i) \rightarrow (W_i, e_i)$.

- ▷ By definition this holds for d_0 and e_0 (both are constantly zero).
- ▷ If the property holds for an ordinal i , then in order to show it for $i + 1$ we recall that $z = p_{\lambda, \lambda+1}^{-1}$. Hence we have by properties of the connection morphisms $Fp^i = Fp_{i,\lambda} = p_{i+1, \lambda+1} = p_{i+1, \lambda} \circ p_{\lambda, \lambda+1} = p^{i+1} \circ z^{-1}$ and thus $Fp^i \circ z = p^{i+1}$. Since by hypothesis $p^i: (Z, d_i) \rightarrow (W_i, e_i)$ is an isometry, the fact that isometries are preserved by \bar{F} implies that $\bar{F}p^i: (FZ, d_i^F) \rightarrow (W_{i+1}, e_{i+1})$ is an isometry. Furthermore $z: (Z, d_{i+1}) \rightarrow (FZ, d_i^F)$ is an isometry by definition of the d_i (see Theorem 5.5.1, page 183). Hence also their composition $p^{i+1} = Fp^i \circ z$ is an isometry.
- ▷ For a limit ordinal j we calculate for $x, y \in Z$

$$\begin{aligned} e_j(p^j(x), p^j(y)) &= \sup_{i < j} e_i((p_{i,j} \circ p^j)(x), (p_{i,j} \circ p^j)(y)) = \sup_{i < j} e_i(p^i(x), p^i(y)) \\ &= \sup_{i < j} d_i(x, y) = d_j(x, y) \end{aligned}$$

and thus also $p^j: (Z, d_j) \rightarrow (W_j, e_j)$ is an isometry.

Let λ be the ordinal for which the final chain converges. We assume that $\lambda \geq \theta$, otherwise set $\lambda = \theta$ (if the final chain converges in θ steps it also converges for all larger ordinals), thus $d_\lambda = d_\theta$. Now let $x, y \in Z$ with $d_\theta(x, y) = d_\lambda(x, y) = 0$. This implies $e_i(p^i(x), p^i(y)) = 0$ for all ordinals $i \leq \lambda$. Since all e_i are metrics, we infer that $p^i(x) = p^i(y)$ for all ordinals i . With the same reasoning as above (where we proved that e_j is a metric for limit ordinals j) this implies that x and y are equal. \square

Corollary 5.5.11 (Bisimilarity Metric) Let $\bar{F}: \text{PMet} \rightarrow \text{PMet}$ be a lifting of a functor $F: \text{Set} \rightarrow \text{Set}$ which has a final coalgebra. Assume that

1. \bar{F} preserves isometries,
2. \bar{F} preserves metrics,
3. the final chain for F converges, and
4. F preserves weak pullbacks.

Then for every coalgebra $c: X \rightarrow FX$ and all $x, x' \in X$ we have

$$x \sim_c x' \iff \text{bd}_c(x, x') = 0.$$

Proof. We already know from Theorem 5.5.6 that $x \sim_c x'$ implies $\text{bd}_c(x, x') = 0$ so we just have to show the converse. Due to our assumptions we can apply Theorem 5.5.10 so $0 = \text{bd}_c(x, x') = d_\theta(\llbracket x \rrbracket_c, \llbracket x' \rrbracket_c)$ implies $\llbracket x \rrbracket_c = \llbracket x' \rrbracket_c$. Since F preserves weak pullbacks we can use Theorem 2.4.15 (page 58) to conclude that $x \sim_c x'$. \square

We will now get back to the examples studied at the beginning of this chapter (Examples 5.3.1 and 5.3.3, pages 141 and 142) and discuss in which sense they are instances of our framework.

Example 5.5.12 (Bisimilarity Pseudometric for Probabilistic Systems) In order to model the discounted behavioral distance for purely probabilistic systems as given in Example 5.3.1 (page 141) in our framework, we set $\top = 1$ and proceed to lift the following three functors: we first consider the identity functor Id with evaluation map $\text{ev}_{\text{Id}}: [0, 1] \rightarrow [0, 1]$, $\text{ev}_{\text{Id}}(z) = c \cdot z$ in order to integrate the discount (Example 5.4.29, page 164). Then, we take the coproduct with the singleton metric space (Definition 5.4.57 and Lemmas 5.4.59 and 5.4.60, pages 180 ff.). The combination of the two functors yields the discrete version of the refusal functor of Franck van Breugel and James Worrel [vBW06], namely $\bar{\mathcal{R}}(X, d) = (X + \mathbb{1}, \hat{d})$ where \hat{d} is the coproduct pseudometric taken from Example 5.3.1. Finally, we lift the probability distribution functor \mathcal{D} to obtain $\bar{\mathcal{D}}$ (Example 5.4.9, page 149). All functors satisfy the Kantorovich-Rubinstein duality and preserve metrics.

It is easy to see that $\bar{\mathcal{D}}(\bar{\mathcal{R}}(X, d)) = (\mathcal{D}(X + \mathbb{1}), \bar{d})$, where \bar{d} is defined as in Example 5.3.1). Then, the least solution of $d(x, y) = \bar{d}(c(x), c(y))$ can be computed as in Theorem 5.5.7.

Example 5.5.13 (Bisimilarity Pseudometric for Metric Transition Systems) As in Example 5.3.3 we consider metric transition systems which we identified as the coalgebras

$$c: S \rightarrow M_1 \times \cdots \times M_n \times \mathcal{P}_f(S)$$

where S is a finite set of states and (M_i, d_i) are pseudometric spaces. If, for $i \in \{1, \dots, n\}$, $\pi_i: M_1 \times \dots \times M_n \times \mathcal{P}_f(S) \rightarrow M_i$ and $\pi_{n+1}: M_1 \times \dots \times M_n \times \mathcal{P}_f(S) \rightarrow \mathcal{P}_f(S)$ are the projections of the product, then each state $s \in S$ is assigned a valuation function $[s]: \{1, \dots, n\} \rightarrow \cup_{r=1}^n M_r$ where, of course, $[s](i) = \pi_i(c(S))$, and the set $\pi_{n+1}(c(S))$ of successor states.

To obtain behavioral distances for metric transition systems using our framework we set $\top = \infty$. Moreover, analogously to the product bifunctor of Definition 5.4.52 we can equip the product multifunctor $P: \text{Set}^{n+1} \rightarrow \text{Set}$, $P(X_1, \dots, X_n) = X_1 \times \dots \times X_n$, $P(f_1, \dots, f_n) = f_1 \times \dots \times f_n$ with the evaluation function $\text{ev}_P: [0, \infty]^{n+1} \rightarrow [0, \infty]$ where $\text{ev}_P(r_1, \dots, r_{n+1}) = \max\{r_1, \dots, r_{n+1}\}$ which is a natural generalization of the function presented in Lemma 5.4.54. As in that lemma, this function is well-behaved in the sense of Definition 5.4.46 and analogously to Lemma 5.4.55 we can easily see that duality holds and we obtain the categorical product pseudometric, i.e., for given pseudometric spaces (X_i, d_i) the new pseudometric

$$d^F: X_1 \times \dots \times X_{n+1} \rightarrow [0, \infty], \quad d^F = \max\{d_1, \dots, d_{n+1}\}.$$

Let \bar{P} be the corresponding lifted multifunctor. We instantiate the given pseudometric spaces (M_i, d_i) as fixed parameters and obtain the endofunctor $\bar{F}: \text{PMet} \rightarrow \text{PMet}$ with

$$\bar{F}(X, d) = \bar{P}((M_1, d_1), \dots, (M_n, d_n) \times \bar{\mathcal{P}}_f(X, d))$$

where $\bar{\mathcal{P}}_f$ is the lifting of the powerset functor using the evaluation function $\max: \mathcal{P}_f([0, \infty]) \rightarrow [0, \infty]$ with $\max \emptyset = 0$ as presented in Example 5.4.31. Then, via Theorem 5.5.7, we obtain exactly the least solution of

$$d(s, t) = \max \left\{ \bar{p}d([s], [t]), \max_{s' \in \tau(s)} \min_{t' \in \tau(t)} d(s', t'), \max_{t' \in \tau(t)} \min_{s' \in \tau(s)} d(s', t') \right\}$$

as in (5.3.1) in Example 5.3.3. Except for the fact that we allow $+\infty$ and consider only undirected (symmetric) pseudometrics, this is exactly the branching distance bd^{Ss} as defined by Luca de Alfaro, Marco Faella, and Mari  lle Stoelinga [dAFSo9, Definition 13].

5.6 Compositionality of Liftings

In the remainder of this chapter we want to turn our attention to trace pseudometrics. Since we plan to apply the generalized powerset construction we will have to lift not only functors but also monads from Set to PMet . As a

preparation for that we now study *compositionality* of functor liftings, i.e., we set off to identify some sufficient conditions ensuring $\overline{F} \overline{G} = \overline{FG}$. Unfortunately, this seems to be a quite difficult question in this general setting so our main result only treats the Wasserstein lifting and requires the existence of optimal couplings. However, whenever it can be applied it allows us to reason modularly and, consequently, to simplify the proofs needed for the treatment of our examples.

As further preparation for the trace pseudometric we will also consider two examples involving the finite powerset monad where optimal couplings do not always exist and manually prove that compositionality holds for these specific cases.

5.6.1 Compositionality for Endofunctors

Given functors $F, G: \text{Set} \rightarrow \text{Set}$ with evaluation functions ev_F and ev_G , we can easily construct an evaluation function for the composition FG as follows.

Definition 5.6.1 (Composition of Evaluation Functions) Let F and G be endofunctors on Set with evaluation functions ev_F and ev_G . We define the composition of ev_F and ev_G to be the evaluation function $\text{ev}_F * \text{ev}_G: FG[0, \top] \rightarrow [0, \top]$ for the composed functor FG via $\text{ev}_F * \text{ev}_G := \widetilde{F}\text{ev}_G = \text{ev}_F \circ \text{Fev}_G$.

Our first step will be to show that, whenever F and G preserve weak pullbacks, well-behavedness is inherited.

Theorem 5.6.2 (Well-Behavedness of Composed Evaluation Function) Let F, G be endofunctors on Set with evaluation functions ev_F, ev_G . If both functors preserve weak pullbacks and both evaluation functions are well-behaved then also $\text{ev}_F * \text{ev}_G$ is well-behaved.

We will split the proof into two technical lemmas. The first of these just summarizes some useful rules for calculations.

Lemma 5.6.3 Let F, G be endofunctors on Set with evaluation functions ev_F, ev_G and $\alpha := \langle G\pi_1, G\pi_2 \rangle$ (i.e., the unique mediating arrow into the product $GX \times GX$, where $\pi_i: X^2 \rightarrow X$ are the projections) and (X, d) an arbitrary pseudometric space. Then the following holds.

1. We always have $\widetilde{G}d \geq d^{\downarrow G} \circ \alpha$ and if ev_G satisfies Conditions W1 and W2 we also have $\widetilde{G}d \geq d^{\uparrow G} \circ \alpha$
2. $\forall t_1, t_2 \in FGX: t \in \Gamma_{FG}(t_1, t_2) \implies Fa(t) \in \Gamma_F(t_1, t_2)$.

3. If F and G preserve weak pullbacks then so does FG .
4. For any $f \in \text{Set}/[0, \top]$ we have $\widetilde{FG}f = \widetilde{F}(\widetilde{G}f)$.

Proof. We first of all observe that α is the unique mediating arrow into the product $GX \times GX$ making the following diagram commute, where $\pi_i: X^2 \rightarrow X$ and $\tau_i: (GX)^2 \rightarrow GX$ are the respective projections.

$$\begin{array}{ccccc}
 & & G(X \times X) & & \\
 & \swarrow^{G\pi_1} & \downarrow \alpha = \langle G\pi_1, G\pi_2 \rangle & \searrow^{G\pi_2} & \\
 GX & \xleftarrow{\tau_1} & GX \times GX & \xrightarrow{\tau_2} & GX
 \end{array}$$

1. Let $s \in G(X \times X)$ and define $s_i := G\pi_i(s) = \tau_i \circ \alpha(s)$. Then by definition $s \in \Gamma_G(s_1, s_2)$ and we conclude $\widetilde{G}d(s) \geq \inf \left\{ \widetilde{G}d(s') \mid s' \in \Gamma_G(s_1, s_2) \right\} = d^{\downarrow G}(s_1, s_2) = d^{\downarrow G}(\tau_1 \circ \alpha(s), \tau_2 \circ \alpha(s)) = d^{\downarrow G} \circ \alpha(s)$. Since we always have $d^{\downarrow G} \geq d^{\uparrow G}$ as shown in Theorem 5.4.27, the statement follows.
2. We compute $F\tau_i(F\alpha(t)) = F(\tau_i \circ \alpha)(t) = F(G\pi_i)(t) = FG\pi_i = t_i$.
3. This is indeed clear by definition.
4. Let $f: X \rightarrow [0, \top]$, then $\widetilde{FG}f = \text{ev}_F * \text{ev}_G \circ FGf = \text{ev}_F \circ \text{Fev}_G \circ FGf = \text{ev}_F \circ F(\text{ev}_G \circ Gf) = \widetilde{F}(\widetilde{G}f)$. \square

We can now use these calculations to prove the second lemma which already finishes the proof of the inheritance of well-behavedness.

Lemma 5.6.4 Let F, G be functors with evaluation functions ev_F and ev_G . Then the following holds.

1. If \widetilde{F} and \widetilde{G} are monotone (Condition W_1), then so is the evaluation functor \widetilde{FG} with respect to the composed evaluation function $\text{ev}_F * \text{ev}_G$.
2. If G preserves weak pullbacks, ev_G is well-behaved and \widetilde{F} is monotone (Condition W_1) then $\text{ev}_F * \text{ev}_G$ satisfies Condition W_2 of Definition 5.4.14.
3. If F preserves weak pullbacks and ev_F, ev_G satisfy Condition W_3 of well-behavedness, then also $\text{ev}_F * \text{ev}_G$ satisfies Condition W_3 of Definition 5.4.14.

Proof. 1. Let $f, g: X \rightarrow [0, \top]$ with $f \leq g$, then by monotonicity of ev_G we have $\widetilde{G}f \leq \widetilde{G}g$ and using monotonicity of ev_F we get $\widetilde{FG}f = \widetilde{F}(\widetilde{G}f) \leq \widetilde{F}(\widetilde{G}g) = \widetilde{FG}g$.

- Let $\pi_i: X^2 \rightarrow X$ be the projections of the product. For $t \in FG([0, T]^2)$ we define $t_i := FG\pi_i(t) \in FG[0, T]$. By definition $t \in \Gamma_{FG}(t_1, t_2)$ so Lemma 5.6.3 (page 194) tells us $Fa(t) \in \Gamma_F(t_1, t_2)$ for $a := \langle G\pi_1, G\pi_2 \rangle$. Moreover, since $ev_G: (G[0, T], d_e^{\uparrow G}) \rightarrow ([0, T], d_e)$ is nonexpansive (by definition of the Kantorovich pseudometric), we can apply Lemma 5.4.26 (page 162) to obtain the inequality

$$\begin{aligned} d_e((ev_F * ev_G)(t_1), ev_F * ev_G(t_2)) &= d_e(\tilde{F}ev_G(t_1), \tilde{F}ev_G(t_2)) \\ &\leq \tilde{F}d_e^{\uparrow G}(Fa(t)) = \tilde{F}(d_e^{\uparrow G} \circ a)(t). \end{aligned}$$

By Lemma 5.6.3 we have $d_e^{\uparrow G} \circ a \leq \tilde{G}d_e$ and using monotonicity of \tilde{F} we can continue our inequality with $\tilde{F}(d_e^{\uparrow G} \circ a)(t) \leq \tilde{F}(\tilde{G}d_e)(t) = \tilde{F}\tilde{G}d_e(t)$ which concludes the proof!

- Using Lemma 5.4.17 (page 153) we just have to show that the following diagram is a weak pullback.

$$\begin{array}{ccccc} & & \text{!}_{FG\{0\}} & & \\ & \text{FG}\{0\} & \xrightarrow{\quad} & F\{0\} & \xrightarrow{\quad} & \{0\} \\ & \downarrow FGi & \text{F!}_{G\{0\}} & \downarrow Fi & \text{!}_{F\{0\}} & \downarrow i \\ & FG[0, T] & \xrightarrow{\quad Fev_G \quad} & F[0, T] & \xrightarrow{\quad ev_F \quad} & [0, T] \\ & & & & & \text{ev}_F * \text{ev}_G \end{array}$$

Lemma 5.4.17 tells us that the right square is a weak pullback and since F preserves weak pullbacks also the left square is. The outer part is thus necessarily a weak pullback again yielding by Lemma 5.4.17 that $ev_F * ev_G$ satisfies Condition W_3 . \square

This lemma concludes the proof of Theorem 5.6.2. In the light of this result we know that, whenever we start with pullback preserving functors F, G along with well-behaved evaluation functions ev_F, ev_G , the Wasserstein function for FG (with respect to $ev_F * ev_G$) is a pseudometric (see Theorem 5.4.20, page 157) so we can safely talk about *the* Wasserstein lifting of FG and study compositionality.

We will now show that a sufficient criterion for compositionality of the Wasserstein lifting is the existence of optimal couplings for G . Again we start with a technical lemma which also contains a small statement about the Kantorovich lifting.

Lemma 5.6.5 Let F and G be endofunctors on Set together with evaluation functions $\text{ev}_F: F[0, \top] \rightarrow [0, \top]$, $\text{ev}_G: G[0, \top] \rightarrow [0, \top]$. We define $\text{ev}_F * \text{ev}_G := \text{ev}_F \circ \text{Fev}_G$. Then the following properties hold for every pseudometric space (X, d) .

1. $d^{\uparrow FG} \leq (d^{\uparrow G})^{\uparrow F}$.
2. If ev_F and ev_G satisfy Conditions W1 and W2 then $d^{\downarrow FG} \geq (d^{\downarrow G})^{\downarrow F}$.
3. If for all $t_1, t_2 \in FGX$ there is a function $\nabla(t_1, t_2): \Gamma_F(t_1, t_2) \rightarrow \Gamma_{FG}(t_1, t_2)$ such that $\widetilde{FG}d \circ \nabla(t_1, t_2) = \widetilde{F}d^{\downarrow G}$ then $d^{\downarrow FG} \leq (d^{\downarrow G})^{\downarrow F}$.

Proof. Let $t_1, t_2 \in FGX$.

1. Recall that $d^{\uparrow G}$ is the smallest pseudometric such that for every nonexpansive function $f: (X, d) \rightarrow ([0, \top], d_e)$ also $\widetilde{G}f: (GX, d^{\uparrow G}) \rightarrow ([0, \top], d_e)$ is nonexpansive (see remark in the beginning of Section 5.4.1 on page 145). Moreover, $\widetilde{FG}f = \widetilde{F}(\widetilde{G}f)$ by Lemma 5.6.3. Thus

$$\begin{aligned} d^{\uparrow FG}(t_1, t_2) &= \sup \left\{ d_e \left(\widetilde{FG}f(t_1), \widetilde{FG}f(t_2) \right) \mid f: (X, d) \rightarrow ([0, \top], d_e) \right\} \\ &= \sup \left\{ d_e \left(\widetilde{F}(\widetilde{G}f)(t_1), \widetilde{F}(\widetilde{G}f)(t_2) \right) \mid f: (X, d) \rightarrow ([0, \top], d_e) \right\} \\ &\leq \sup \left\{ d_e \left(\widetilde{F}(g)(t_1), \widetilde{F}(g)(t_2) \right) \mid g: (GX, d^{\uparrow G}) \rightarrow ([0, \top], d_e) \right\} \\ &= (d^{\uparrow G})^{\uparrow F}(t_1, t_2) \end{aligned}$$

2. Lemma 5.6.3 tells us $\widetilde{G}d \geq d^{\downarrow G} \circ \alpha$ and for any coupling $t \in \Gamma_{FG}(t_1, t_2)$ we have $\text{Fa}(t) \in \Gamma_F(t_1, t_2)$. Using these facts and the monotonicity of \widetilde{F} we obtain:

$$\begin{aligned} d^{\downarrow FG}(t_1, t_2) &= \inf \left\{ \widetilde{FG}d(t) \mid t \in \Gamma_{FG}(t_1, t_2) \right\} = \inf \left\{ \widetilde{F}(\widetilde{G}d)(t) \mid t \in \Gamma_{FG}(t_1, t_2) \right\} \\ &\geq \inf \left\{ \widetilde{F}(d^{\downarrow G} \circ \alpha)(t) \mid t \in \Gamma_{FG}(t_1, t_2) \right\} \\ &= \inf \left\{ \widetilde{F}d^{\downarrow G}(\text{Fa}(t)) \mid t \in \Gamma_{FG}(t_1, t_2) \right\} \\ &\geq \inf \left\{ \widetilde{F}d^{\downarrow G}(t') \mid t' \in \Gamma_F(t_1, t_2) \right\} = (d^{\downarrow G})^{\downarrow F}(t_1, t_2) \end{aligned}$$

3. Using $\nabla(t_1, t_2)$ we compute

$$\begin{aligned} d^{\downarrow FG}(t_1, t_2) &= \inf \left\{ \widetilde{FG}d(t') \mid t' \in \Gamma_{FG}(t_1, t_2) \right\} \\ &\leq \inf \left\{ \widetilde{FG}d(\nabla(t_1, t_2)(t)) \mid t \in \Gamma_F(t_1, t_2) \right\} \\ &= \inf \left\{ \widetilde{F}d^{\downarrow G}(t) \mid t \in \Gamma_F(t_1, t_2) \right\} = (d^{\downarrow G})^{\downarrow F}(t_1, t_2) \end{aligned}$$

which concludes the proof. □

With this result at hand we can now prove the compositionality for the Wasserstein lifting.

Theorem 5.6.6 (Compositionality of the Wasserstein Lifting) Let F, G be weak pullback preserving endofunctors on \mathbf{Set} with well-behaved evaluation functions ev_F, ev_G and (X, d) be a pseudometric space. If for all $t_1, t_2 \in GX$ there is an optimal G -coupling $\gamma(t_1, t_2) \in \Gamma_G(t_1, t_2)$ such that $d^{\downarrow G}(t_1, t_2) = \widetilde{G}d(\gamma(t_1, t_2))$ then we have the equality $d^{\downarrow FG} = (d^{\downarrow G})^{\downarrow F}$.

Proof. From Lemma 5.6.5.2 we know $d^{\downarrow FG} \geq (d^{\downarrow G})^{\downarrow F}$. We just have to show the other inequality. By our requirement we have a function $\gamma: GX \times GX \rightarrow G(X \times X)$, such that $d^{\downarrow G} = \widetilde{G}d \circ \gamma$. Moreover, let $\pi_i: X^2 \rightarrow X$ and $\tau_i: (GX)^2 \rightarrow GX$ be the projections of the product then γ satisfies $G\pi_i \circ \gamma = \tau_i$. Given $t_1, t_2 \in FGX$ and $t \in \Gamma_F(t_1, t_2)$, we define $\nabla(t_1, t_2)(t) = F\gamma(t)$, then this satisfies the conditions of Lemma 5.6.5.3. First, we have $F\gamma(t) \in \Gamma_{FG}(t_1, t_2)$ because $FG\pi_i(F\gamma(t)) = F(G\pi_i \circ \gamma)(t) = F\tau_i(t) = t_i$. Moreover

$$\begin{aligned} \widetilde{FG}d(F\gamma(t)) &= \text{ev}_F * \text{ev}_G \circ F(Gd \circ \gamma(t)) = \text{ev}_F \circ F\text{ev}_G \circ F(Gd \circ \gamma)(t) \\ &= \text{ev}_F \circ F(\widetilde{G}d \circ \gamma)(t) = \text{ev}_F \circ Fd^{\downarrow G}(t) = \widetilde{F}d^{\downarrow G}(t) \end{aligned}$$

so Lemma 5.6.5.3 yields $d^{\downarrow FG} \leq (d^{\downarrow G})^{\downarrow F}$. \square

This criterion will sometimes turn out to be useful for our later results. Nevertheless it provides just a sufficient condition for compositionality as the following examples show.

Example 5.6.7 (Compositionality for the Distribution Functor) We consider the distribution functor (with finite support) \mathcal{D}_f of Example 2.3.12 with the evaluation function defined in Example 5.4.9. For any pseudometric space (X, d) we have $d^{\downarrow \mathcal{D}_f \mathcal{D}_f} = (d^{\downarrow \mathcal{D}_f})^{\downarrow \mathcal{D}_f}$ by Theorem 5.6.6 because optimal couplings always exist.

Example 5.6.8 (Compositionality for the Finite Powerset Functor) We consider the finite powerset functor \mathcal{P}_f of Example 2.3.11 with the evaluation function defined in Example 5.4.16. We claim that for any pseudometric space (X, d) we have $d^{\downarrow \mathcal{P}_f \mathcal{P}_f} = (d^{\downarrow \mathcal{P}_f})^{\downarrow \mathcal{P}_f}$ although \mathcal{P}_f -couplings do not always exist. To verify this, we recall from Lemma 5.6.5.2 that

$$d^{\downarrow \mathcal{P}_f \mathcal{P}_f} \geq (d^{\downarrow \mathcal{P}_f})^{\downarrow \mathcal{P}_f} \quad (5.6.1)$$

holds. We now show that we always have equality. Let (X, d) be a pseudometric space and $T_1, T_2 \in \mathcal{P}_f \mathcal{P}_f X$. We distinguish three cases:

1. If $T_1 = T_2 = \emptyset$ we know by reflexivity that both sides of (5.6.1) are 0.
2. If $T_1 = \emptyset \neq T_2$ or $T_1 \neq \emptyset = T_2$ we know from Example 5.4.31 that $\Gamma_{\mathcal{P}_f}(T_1, T_2) = \emptyset$ and therefore $(d^{\downarrow \mathcal{P}_f})^{\downarrow \mathcal{P}_f}(T_1, T_2) = \top$ and thus (5.6.1) is necessarily an equality because the left hand side can never exceed \top .
3. Let $T_1, T_2 \neq \emptyset$. We know from Example 5.4.31 that we have an optimal coupling $T^* \in \Gamma_{\mathcal{P}_f}(T_1, T_2)$, say $T^* = \{(V_{j1}, V_{j2}) \in \mathcal{P}_f X \times \mathcal{P}_f X \mid j \in J\}$ for a suitable index set J . Then, using the projections $\pi_i: (\mathcal{P}_f X)^2 \rightarrow \mathcal{P}_f X$, we have $T_i = \mathcal{P}_f \pi_i(T^*) = \pi_i[T^*] = \{\pi_i((V_{j1}, V_{j2})) \mid j \in J\} = \{V_{ji} \mid j \in J\}$. By optimality we thus have:

$$(d^{\downarrow \mathcal{P}_f})^{\downarrow \mathcal{P}_f}(T_1, T_2) = \widetilde{\mathcal{P}_f} d^{\downarrow \mathcal{P}_f}(T^*) = \max d^{\downarrow \mathcal{P}_f}[T^*] = \max_{j \in J} d^{\downarrow \mathcal{P}_f}(V_{j1}, V_{j2}). \quad (5.6.2)$$

We will make another case distinction:

- 3.1. If there is an index $j' \in J$ such that $\Gamma_{\mathcal{P}_f}(V_{j'1}, V_{j'2}) = \emptyset$, we apparently have $d^{\downarrow \mathcal{P}_f}(V_{j'1}, V_{j'2}) = \top$ and by (5.6.2) also $(d^{\downarrow \mathcal{P}_f})^{\downarrow \mathcal{P}_f}(T_1, T_2) = \top$ which again shows that (5.6.1) is an equality.
- 3.2. Otherwise we can take optimal couplings $V_j^* \in \Gamma_{\mathcal{P}_f}(V_{j1}, V_{j2})$ (see Example 5.4.31, page 166). Continuing (5.6.2) we have

$$(d^{\downarrow \mathcal{P}_f})^{\downarrow \mathcal{P}_f}(T_1, T_2) = \max_{j \in J} \widetilde{\mathcal{P}_f} d(V_j^*) = \max_{j \in J} \max d[V_j^*] \quad (5.6.3)$$

We define $T := \{V_j^* \mid j \in J\} \in \mathcal{P}_f \mathcal{P}_f(X \times X)$ and calculate for the projections $\pi_i: X \times X \rightarrow X$

$$\mathcal{P}_f \mathcal{P}_f \pi_i(T) = \mathcal{P}_f \pi_i[T] = \{\mathcal{P}_f \pi_i(V_j^*) \mid j \in J\} = \{V_{ji} \mid j \in J\} = T_i$$

and thus $T \in \Gamma_{\mathcal{P}_f \mathcal{P}_f}(T_1, T_2)$. Moreover we have

$$\begin{aligned} d^{\downarrow \mathcal{P}_f \mathcal{P}_f}(T_1, T_2) &\leq \widetilde{\mathcal{P}_f \mathcal{P}_f} d(T) = \max \left((\mathcal{P}_f \max)(\mathcal{P}_f \mathcal{P}_f d(T)) \right) \\ &= \max \left(\max [(\mathcal{P}_f d)[T]] \right) = \max \left(\max [\{d[V_j^*] \mid j \in J\}] \right) \\ &= \max \left(\{ \max d[V_j^*] \mid j \in J \} \right) \\ &= \max_{j \in J} \max d[V_j^*]. \end{aligned} \quad (5.6.4)$$

Thus using this, (5.6.3) and (5.6.1) we conclude that

$$d^{\downarrow \mathcal{P}_f \mathcal{P}_f}(T_1, T_2) \leq \max_{j \in J} \max d[V_j^*] = (d^{\downarrow \mathcal{P}_f})^{\downarrow \mathcal{P}_f}(T_1, T_2) \leq d^{\downarrow \mathcal{P}_f \mathcal{P}_f}(T_1, T_2)$$

which proves equality also in this last case.

We conclude our study of compositionality for endofunctors with another example for which we again have to show compositionality separately. This result will later turn out to be helpful to obtain trace pseudometrics for non-deterministic automata and we can use the same approach as in the previous example.

Example 5.6.9 As in Example 5.4.35 (page 169) we equip the machine functor with the evaluation function $\text{ev}_{M_2}: 2 \times [0, 1]^A \rightarrow [0, 1]$, $(o, s) \mapsto c \cdot \text{ev}_1(s)$ where $c \in]0, 1]$ and ev_1 is one of the evaluation functions for the input functor from Example 5.4.34. Moreover, for the powerset functor we use the maximum as evaluation function (see Example 5.4.16). We claim that, although couplings for M_2 do not always exist, we have $d^{\downarrow \mathcal{P}_f M_2} = (d^{\downarrow M_2})^{\downarrow \mathcal{P}_f}$.

To prove this claim, we adapt the approach employed in Example 5.6.8. We know from Lemma 5.6.5.2 that

$$d^{\downarrow \mathcal{P}_f M_2} \geq (d^{\downarrow M_2})^{\downarrow \mathcal{P}_f} \quad (5.6.5)$$

holds. We now show that we always have equality. Let (X, d) be a pseudometric space and $T_1, T_2 \in \mathcal{P}_f M_2 2 = \mathcal{P}_f(2 \times X^A)$. We distinguish three cases:

1. If $T_1 = T_2 = \emptyset$ we know by reflexivity that both sides of (5.6.5) are 0.
2. If $T_1 = \emptyset \neq T_2$ or $T_1 \neq \emptyset = T_2$ we know from Example 5.4.31 that $\Gamma_{\mathcal{P}_f}(T_1, T_2) = \emptyset$ and therefore $(d^{\downarrow M_2})^{\downarrow \mathcal{P}_f}(T_1, T_2) = \top$ and thus (5.6.5) is an equality because the left hand side never exceeds \top .
3. Let $T_1, T_2 \neq \emptyset$. We know from Example 5.4.31 that we have an optimal coupling $T^* \in \Gamma_{\mathcal{P}_f}(T_1, T_2)$, say $T^* = \{((o_{j1}, s_{j1}), (o_{j2}, s_{j2})) \in M_2 X \times M_2 X \mid j \in J\}$ for a suitable index set J . Then using the projections $\pi_i: M_2 X \times M_2 X \rightarrow M_2 X$ we have $T_i = \mathcal{P}_f \pi_i(T^*) = \pi_i[T^*] = \{(o_{ji}, s_{ji}) \mid j \in J\} = \{(o_{ji}, s_{ji}) \mid j \in J\}$. By optimality we thus have

$$\begin{aligned} (d^{\downarrow M_2})^{\downarrow \mathcal{P}_f}(T_1, T_2) &= \tilde{\mathcal{P}}_f d^{\downarrow M_2}(T^*) = \max d^{\downarrow M_2}[T^*] \\ &= \max_{j \in J} d^{\downarrow M_2}((o_{j1}, s_{j1}), (o_{j2}, s_{j2})). \end{aligned} \quad (5.6.6)$$

We will make another case distinction:

- 3.1. If there is a $j' \in J$ such that $\Gamma_{M_2}((o_{j'1}, s_{j'1}), (o_{j'2}, s_{j'2})) = \emptyset$ (which is the case if and only if $o_{j'1} \neq o_{j'2}$), we have $d^{\downarrow M_2}((o_{j'1}, s_{j'1}), (o_{j'2}, s_{j'2})) = \top$ and using (5.6.6) also $(d^{\downarrow M_2})^{\downarrow \mathcal{P}_f}(T_1, T_2) = \top$ which again shows that (5.6.5) is an equality.

3.2. Otherwise for every index $j \in J$ we can take the coupling $(o_{j1}, \langle s_{j1}, s_{j2} \rangle) \in \Gamma_{M_2}((o_{j1}, s_{j1}), (o_{j2}, s_{j2}))$ which is unique and thus optimal. Continuing (5.6.6) we have

$$\begin{aligned}
 (d^{\downarrow M_2})^{\downarrow \mathcal{P}_f}(T_1, T_2) &= \max_{j \in J} \widetilde{M_2} d(o_{j1}, \langle s_{j1}, s_{j2} \rangle) \\
 &= \max_{j \in J} \text{ev}_{M_2} \left((\text{id}_2 \times d^A)(o_{j1}, \langle s_{j1}, s_{j2} \rangle) \right) \\
 &= \max_{j \in J} \text{ev}_{M_2} (o_{j1}, d \circ \langle s_{j1}, s_{j2} \rangle) \\
 &= c \cdot \max_{j \in J} \text{ev}_I(d \circ \langle s_{j1}, s_{j2} \rangle) \tag{5.6.7}
 \end{aligned}$$

We define

$$T := \{(o_{j1}, \langle s_{j1}, s_{j2} \rangle) \mid j \in J\} \in \mathcal{P}_f M_2(X \times X) = \mathcal{P}_f(2 \times (X \times X)^A).$$

We calculate for the projections $\pi_i: X \times X \rightarrow X$

$$\mathcal{P}_f M_2 \pi_i(T) = (\text{id}_2 \times \pi_i^A)[T] = \{(o_{j1}, s_{ji}) \mid j \in J\} = T_i$$

and thus $T \in \Gamma_{\mathcal{P}_f M_2}(T_1, T_2)$. Moreover we have

$$\begin{aligned}
 d^{\downarrow \mathcal{P}_f M_2}(T_1, T_2) &\leq \widetilde{\mathcal{P}_f M_2} d(T) = \text{ev}_{\mathcal{P}_f} \circ \mathcal{P}_f \text{ev}_{M_2} \circ \mathcal{P}_f M_2 d(T) \\
 &= \max (\mathcal{P}_f (\text{ev}_{M_2} \circ M_2 d)(T)) = \max ((\text{ev}_{M_2} \circ M_2 d)[T]) \\
 &= \max (\text{ev}_{M_2} [(\text{id}_2 \times d^A)[T]]) \\
 &= \max (\text{ev}_{M_2} [\{(\text{id}_2 \times d^A)(o_{j1}, \langle s_{j1}, s_{j2} \rangle) \mid j \in J\}]) \\
 &= \max_{j \in J} \text{ev}_{M_2} (o_{j1}, d \circ \langle s_{j1}, s_{j2} \rangle) \\
 &= c \cdot \max_{j \in J} \text{ev}_I(d \circ \langle s_{j1}, s_{j2} \rangle) \tag{5.6.8}
 \end{aligned}$$

thus using this, (5.6.7) and (5.6.5) we conclude that

$$\begin{aligned}
 d^{\downarrow \mathcal{P}_f M_2}(T_1, T_2) &\leq c \cdot \max_{j \in J} \text{ev}_I(d \circ \langle s_{j1}, s_{j2} \rangle) \\
 &= (d^{\downarrow M_2})^{\downarrow \mathcal{P}_f}(T_1, T_2) \leq d^{\downarrow \mathcal{P}_f M_2}(T_1, T_2)
 \end{aligned}$$

which proves equality.

5.6.2 Compositionality for Multifunctors

We conclude the analysis of compositionality with a short explanation on how our theory extends to multifunctors.

For $n \in \mathbb{N}$ we denote by $[n] := \{1, \dots, n\} \subseteq \mathbb{N}$ the set of all positive natural numbers less than or equal to n . Now let $n_i \in \mathbb{N}$ for all $i \in [n]$ and $F: \text{Set}^n \rightarrow \text{Set}$ and $G_i: \text{Set}^{n_i} \rightarrow \text{Set}$ (for $i \in [n]$) be multifunctors with evaluation functions $\text{ev}_F: F([0, \top]^n) \rightarrow [0, \top]$ and $\text{ev}_{G_i}: G_i([0, \top]^{n_i}) \rightarrow [0, \top]$. We define $N := \sum_{i=1}^n n_i$ and define the functor

$$H := F \circ \prod_{i=1}^n G_i = F \circ (G_1 \times G_2 \times \dots \times G_n): \text{Set}^N \rightarrow \text{Set}$$

Then we can define the evaluation function $\text{ev}_H: H([0, \top]^N) \rightarrow [0, \top]$ by

$$\text{ev}_H := \text{ev}_F \circ F(\text{ev}_{G_1}, \text{ev}_{G_2}, \dots, \text{ev}_{G_n}).$$

In this setting, compositionality of the lifting means that whenever we have N pseudometric spaces (X_i, d_i) the pseudometric $(d_1, \dots, d_N)^H$ is equal to

$$\left((d_1, \dots, d_{n_1})^{G_1}, (d_{n_1+1}, \dots, d_{n_1+n_2})^{G_2} \dots, (d_{N-n_n+1}, \dots, d_N)^{G_n} \right)^F.$$

In the examples in this thesis we will just use the Wasserstein lifting and we only have the following two cases:

1. $n = 1$, $n_1 = 2$ so that $F: \text{Set} \rightarrow \text{Set}$ is an endofunctor with evaluation function $\text{ev}_F: F[0, \top] \rightarrow [0, \top]$ and $G: \text{Set}^2 \rightarrow \text{Set}$ is a bifunctor with evaluation function $\text{ev}_G: G([0, \top], [0, \top]) \rightarrow [0, \top]$. Then we have $N = n_1 = 2$ and obtain the bifunctor $H = F \circ G: \text{Set}^2 \rightarrow \text{Set}$ with evaluation $\text{ev}_H = \text{ev}_F \circ \text{Fev}_G: FG([0, 1], [0, 1]) \rightarrow [0, 1]$. Compositionality means that for an two pseudometric spaces $(X_1, d_1), (X_2, d_2)$ we have $(d_1, d_2)^{\downarrow H} = ((d_1, d_2)^{\downarrow G})^{\downarrow F}$.
2. $n = 2$, $n_1 = n_2 = 1$ so that $F: \text{Set}^2 \rightarrow \text{Set}$ is a bifunctor with evaluation function $\text{ev}_F: F([0, \top], [0, \top]) \rightarrow [0, \top]$ and $G_1, G_2: \text{Set} \rightarrow \text{Set}$ are endofunctors with evaluations $\text{ev}_{G_i}: G_i[0, \top] \rightarrow [0, \top]$. Then we have $N = n_1 + n_2 = 1 + 1 = 2$ and obtain the bifunctor $H = F \circ (G_1 \times G_2): \text{Set}^2 \rightarrow \text{Set}$ with evaluation $\text{ev}_H = \text{ev}_F \circ F(\text{ev}_{G_1}, \text{ev}_{G_2}): F(G_1[0, \top], G_2[0, \top]) \rightarrow [0, \top]$. Compositionality means that for an two pseudometric spaces $(X_1, d_1), (X_2, d_2)$ we have $(d_1, d_2)^{\downarrow H} = (d_1^{\downarrow G_1}, d_2^{\downarrow G_2})^{\downarrow F}$.

The results presented for endofunctors work analogously in the multifunctor case (the proofs can be transferred almost verbatim), so we do not explicitly present them here. Instead, we will use compositionality to obtain the machine bifunctor.

Example 5.6.10 (Machine Bifunctor) Let $I = _{}^A$ be the input functor of Example 2.4.2, Id the identity endofunctor on Set and P be the product bifunctor of Definition 5.4.52. The *machine bifunctor* is the composition $M := P \circ (\text{Id} \times I)$, i.e., the bifunctor $M: \text{Set}^2 \rightarrow \text{Set}$ with

$$M(B, X) := B \times X^A.$$

We compute the composed evaluation function which, of course, depends on the evaluation functions for P and I (for Id we always take $\text{id}_{[0, \top]}$). Let $(o, s) \in [0, \top] \times [0, \top]^A$, then

$$\begin{aligned} \text{ev}_M(o, s) &= \text{ev}_P \circ P(\text{id}_{[0, \top]}, \text{ev}_I)(o, s) \\ &= \text{ev}_P \circ (\text{id}_{[0, \top]} \times \text{ev}_I)(o, s) = \text{ev}_P(o, \text{ev}_I(s)). \end{aligned}$$

By instantiating ev_P and ev_I as in the table below (see also Example 5.4.34 and Lemmas 5.4.53 and 5.4.55), we obtain the corresponding evaluation functions $\text{ev}_M: [0, \top] \times [0, \top]^A \rightarrow [0, \top]$. They are well-behaved due to the fact that all involved functors preserve weak pullbacks and for Id and I there are unique (thus optimal) couplings so we have compositionality by a multifunctor equivalent to Theorem 5.6.2.

Parameters	$\text{ev}_P(r_1, r_2)$	$\text{ev}_I(s)$	$\text{ev}_M(o, s)$
$c_1, c_2 \in]0, 1]$	$\max\{c_1 r_1, c_2 r_2\}$	$\max_{a \in A} s(a)$	$\max\left\{c_1 o, c_2 \max_{a \in A} s(a)\right\}$
$c_1, c_2 \in]0, 1],$ $c_1 + c_2 \leq 1$	$c_1 x_1 + c_2 x_2$	$ A ^{-1} \sum_{a \in A} s(a)$	$c_1 o + c_2 A ^{-1} \sum_{a \in A} s(a)$
$c_1, c_2 \in]0, \infty[,$ $\top = \infty$	$c_1 x_1 + c_2 x_2$	$\sum_{a \in A} s(a)$	$c_1 o + c_2 \sum_{a \in A} s(a)$

Now let $(B, d_B), (X, d)$ be pseudometric spaces. For any $t_1, t_2 \in M(B, X)$ with $t_i = (b_i, s_i) \in B \times X^A$ the unique and therefore necessarily optimal coupling is $t := (b_1, b_2, \langle s_1, s_2 \rangle)$. We compute the Wasserstein distance

$$\begin{aligned} (d_B, d)^{\downarrow M}(t_1, t_2) &= \widetilde{M}(d_B, d)(t) = \text{ev}_M \circ M(d_B, d)(t) \\ &= \text{ev}_M \circ (d_B \times d^A)(b_1, b_2, \langle s_1, s_2 \rangle) \\ &= \text{ev}_M(d_B(b_1, b_2), d \circ \langle s_1, s_2 \rangle). \end{aligned}$$

Thus we obtain in the first case

$$(d_B, d)^{\downarrow M}(t_1, t_2) = \max \left\{ c_1 d_B(b_1, b_2), c_2 \cdot \max_{a \in A} d(s_1(a), s_2(a)) \right\}$$

in the second case

$$(d_B, d)^{\downarrow M}(t_1, t_2) = c_1 d_B(b_1, b_2) + c_2 |A|^{-1} \sum_{a \in A} d(s_1(a), s_2(a))$$

and in the third case

$$(d_B, d)^{\downarrow M}(t_1, t_2) = c_1 d_B(b_1, b_2) + c_2 \sum_{a \in A} d(s_1(a), s_2(a)).$$

Of course one has to choose which of these pseudometrics fits into the respective context. While the first one selects either the distance of the output values or the maximal distance of the successors and neglects the other one, the latter two accumulate the distances. Depending on our maximal element, we have to make sure that we stay within the selected measuring interval $[0, \top]$ by proper scaling of the values.

Usually we will fix the first argument of the machine bifunctor (the set of outputs) and just consider the machine endofunctor $M_B := M(B, _)$ as in Examples 5.6.9 and 5.4.35 (pages 169 and 200). However, for the same reasons as explained before for the product bifunctor, we often need to lift it as bifunctor and then fix the first component of the lifted bifunctor. One notable exception is the case where B is endowed with the discrete metric. Then we have the following result.

Example 5.6.11 As in Example 5.6.9 we equip the machine endofunctor $M_B = M(B, _) = B \times _^A$ with the evaluation function

$$ev_{M_B} : B \times [0, 1]^A, \quad ev_{M_B}(o, s) = c \cdot ev_I(s)$$

where $c \in]0, 1]$ and ev_I is one of the evaluation functions for the input functor from Example 5.4.34 (page 168). We claim that if d_B is the discrete metric on B and if we take

$$ev_{M_B} : [0, 1] \times [0, 1]^A, \quad ev_{M_B}(o, s) = \max\{o, c \cdot ev_I(s)\}$$

then the pseudometric obtained via the bifunctor lifting coincides with the one obtained by endofunctor lifting, i.e., for all pseudometric spaces (X, d) we have $(d_B, d)^{\downarrow M} = d^{\downarrow M_B}$.

In order to prove our claim, we note that given two elements $t_1, t_2 \in B \times X^A$, say $t_i = (o_i, s_i)$, their unique multifunctor M -coupling is $t = (o_1, o_2, \langle s_1, s_2 \rangle)$. We now distinguish two cases.

1. If $o_1 \neq o_2$ no M_B -coupling of t_1, t_2 exists so we have $d^{\downarrow M_B}(t_1, t_2) = 1$ but also $d_B(o_1, o_2) = 1$ so $(d_B, d)^{\downarrow M}(t_1, t_2) = \widetilde{M}(d_B, d)(t) \geq d_B(o_1, o_2) \geq 1$.
2. Otherwise, if $o_1 = o_2$ the unique M_B -coupling of t_1, t_2 is $t' = (o_1, \langle s_1, s_2 \rangle)$ and $d_B(o_1, o_2) = 0$ thus

$$\begin{aligned}
 (d_B, d_e)^{\downarrow M}(t_1, t_2) &= \widetilde{M}(d_B, d)(t) = c_2 \text{ev}_I(d \circ \langle s_1, s_2 \rangle) \\
 &= \text{ev}_{M_B}(o_1, d \circ \langle s_1, s_2 \rangle) = \text{ev}_{M_B}((\text{id}_B \times d^A)(o_1, \langle s_1, s_2 \rangle)) \\
 &= \widetilde{M}_B(t') = d^{\downarrow M_B}(t_1, t_2)
 \end{aligned}$$

which proves our claim.

Thus we can see that lifting the machine functor M_B as endofunctor automatically treats the output set as if it was equipped with the discrete metric.

Let us finish our short excursion to the theory of multifunctor compositionality with another example which shows how the machine bifunctor lifting helps to obtain suitable bisimilarity pseudometrics.

Example 5.6.12 (Bisimilarity Pseudometric for Automata with Real Outputs)

We consider the machine endofunctor with output set $[0, 1]$, i.e., the functor $M_{[0,1]} = [0, 1] \times _^A$ which arises out of the machine bifunctor M by fixing the first component to $[0, 1]$. As maximal distance we set $\top = 1$ and equip the machine bifunctor M with the evaluation function $\text{ev}_M: [0, 1] \times [0, 1]^A \rightarrow [0, 1]$ where

$$\text{ev}_M(o, s) = c_1 o + c_2 |A|^{-1} \sum_{a \in A} s(a)$$

for $c_1, c_2 \in]0, 1[$ such that $c_1 + c_2 \leq 1$ as in Example 5.6.10. Moreover, we recall from Example 2.4.10 (page 54) that the carrier of the final $M_{[0,1]}$ -coalgebra is $[0, 1]^{A^*}$.

If we equip $[0, 1]$ with the Euclidean metric d_e and use our knowledge from Example 5.6.10 we know that for any pseudometric d on $[0, 1]^{A^*}$ we obtain as Wasserstein pseudometric the function

$$\begin{aligned}
 (d_e, d)^{\downarrow F}: \left([0, 1] \times ([0, 1]^{A^*})^A\right)^2 &\rightarrow [0, 1], \text{ with} \\
 (d_e, d)^{\downarrow F}((r_1, s_1), (r_2, s_2)) &= c_1 |r_1 - r_2| + \frac{c_2}{|A|} \cdot \sum_{a \in A} d(s_1(a), s_2(a)).
 \end{aligned}$$

We now want to obtain the final coalgebra for the endofunctor $\overline{M}_{([0,1], d_e)} = \overline{M}([0, 1], d_e, _)$ on PMet which is a lifting of $M_{[0,1]}$ by Lemma 5.4.37. For this

we use the fixed-point equation induced by Theorem 5.5.1 (page 183). It is given by, for $p_1, p_2 \in [0, 1]^{A^*}$, the equation

$$d(p_1, p_2) = c_1 |p_1(\varepsilon) - p_2(\varepsilon)| + \frac{c_2}{|A|} \cdot \sum_{a \in A} d(\lambda w.p_1(aw), \lambda w.p_2(aw)).$$

As in the previous example a simple calculation shows that the function

$$\begin{aligned} d_{[0,1]^{A^*}} : [0, 1]^{A^*} \times [0, 1]^{A^*} &\rightarrow [0, 1], \text{ with} \\ d_{[0,1]^{A^*}}(p_1, p_2) &= c_1 \cdot \sum_{w \in A^*} \left(\frac{c_2}{|A|} \right)^{|w|} |p_1(w) - p_2(w)| \end{aligned}$$

is the least fixed-point of this equation so if we equip $[0, 1]^{A^*}$ with this pseudometric we obtain the final $\overline{M}_{([0,1], d_e)}$ -coalgebra. Thus for a probabilistic automaton $\alpha: X \rightarrow [0, 1] \times X^A$ the bisimilarity pseudometric as given in Definition 5.5.4 (page 187) is the function

$$bd_\alpha: X \times X \rightarrow [0, 1], \quad bd_\alpha(x, y) = c_1 \cdot \sum_{w \in A^*} \left(\frac{c_2}{|A|} \right)^{|w|} |\llbracket x \rrbracket_\alpha(w) - \llbracket y \rrbracket_\alpha(w)|$$

where the unique map into the final coalgebra $\llbracket \cdot \rrbracket_\alpha: X \rightarrow [0, 1]^{A^*}$ maps each state to the function describing the output value of the automaton for each finite word when starting from the respective state.

5.7 Lifting Natural Transformations and Monads

If we have a monad on Set , we can of course use our framework to lift the endofunctor T to a functor \overline{T} on pseudometric spaces. A natural question that arises is, whether we also obtain a monad on pseudometric spaces, i.e., if the components of the unit and the multiplication are nonexpansive with respect to the lifted pseudometrics. In order to answer this question, we first take a closer look at sufficient conditions for lifting natural transformations.

Theorem 5.7.1 (Lifting of a Natural Transformation) Let F, G be endofunctors on Set with evaluation functions ev_F, ev_G and $\lambda: F \Rightarrow G$ be a natural transformation. The following two properties hold for the Kantorovich lifting.

1. If $ev_G \circ \lambda_{[0,1]} \leq ev_F$ then λ_X is nonexpansive for all pseudometric spaces (X, d) , i.e., $d^{\uparrow G} \circ (\lambda_X \times \lambda_X) \leq d^{\uparrow F}$.

2. If $\text{ev}_G \circ \lambda_{[0, \top]} = \text{ev}_F$ then λ_X is an isometry for all pseudometric spaces (X, d) , i.e., $d^{\uparrow G} \circ (\lambda_X \times \lambda_X) = d^{\uparrow F}$.

Moreover, similar properties hold for the Wasserstein lifting.

3. If $\text{ev}_G \circ \lambda_{[0, \top]} \leq \text{ev}_F$ then λ_X is nonexpansive for all pseudometric space (X, d) , i.e., $d^{\downarrow G} \circ (\lambda_X \times \lambda_X) \leq d^{\downarrow F}$.
4. If $\text{ev}_G \circ \lambda_{[0, \top]} = \text{ev}_F$ and the Kantorovich-Rubinstein duality holds for F , i.e., $d^{\uparrow F} = d^{\downarrow F}$, then λ_X is an isometry for all pseudometric spaces, i.e., $d^{\downarrow G} \circ (\lambda_X \times \lambda_X) = d^{\downarrow F}$.

Proof. Let $t_1, t_2 \in FX$.

1. By naturality of λ and $\text{ev}_G \circ \lambda_{[0, \top]} \leq \text{ev}_F$ we obtain for every $f: X \rightarrow [0, \top]$:

$$\tilde{G}f \circ \lambda_X = \text{ev}_G \circ Gf \circ \lambda_X = \text{ev}_G \circ \lambda_{[0, \top]} \circ Ff \leq \text{ev}_F \circ Ff = \tilde{F}f. \quad (5.7.1)$$

Using this we compute

$$d^{\uparrow G}(\lambda_X(t_1), \lambda_X(t_2)) \quad (5.7.2)$$

$$\begin{aligned} &= \sup \left\{ d_e \left(\tilde{G}f(\lambda_X(t_1)), \tilde{G}f(\lambda_X(t_2)) \right) \mid f: (X, d) \rightarrow ([0, \top], d_e) \right\} \\ &\leq \sup \left\{ d_e \left(\tilde{F}f(t_1), \tilde{F}f(t_2) \right) \mid f: (X, d) \rightarrow ([0, \top], d_e) \right\} = d^{\uparrow F}(t_1, t_2). \end{aligned} \quad (5.7.3)$$

2. We just have to replace the inequality by equality in (5.7.1) and (5.7.3).
3. Naturality of λ yields the following equations, where $\pi_i: X \times X \rightarrow X$ are the projections of the product and $d: X \times X \rightarrow [0, \top]$ a pseudometric on X .

$$\lambda_X \circ F\pi_i = G\pi_i \circ \lambda_{X \times X} \quad (5.7.4)$$

$$\lambda_{[0, \top]} \circ Fd = Gd \circ \lambda_{X \times X} \quad (5.7.5)$$

Using (5.7.4), we can see that $\lambda_{X \times X}$ maps every coupling $t \in \Gamma_F(t_1, t_2)$ to a coupling $\lambda_{X \times X}(t) \in \Gamma_G(\lambda_X(t_1), \lambda_X(t_2))$ because $G\pi_i(\lambda_{X \times X}(t)) = \lambda_X(F\pi_i(t)) = \lambda_X(t_i)$. Moreover, by our requirement ($\text{ev}_G \circ \lambda_{[0, \top]} \leq \text{ev}_F$) we obtain

$$\tilde{G}d(\lambda_{X \times X}(t)) = \text{ev}_G \circ Gd \circ \lambda_{X \times X}(t) = \text{ev}_G \circ \lambda_{[0, \top]} \circ Fd(t) \leq \text{ev}_F \circ Fd(t) = \tilde{F}d(t)$$

With these preparations at hand we can finally see that

$$\begin{aligned} d^{\downarrow G}(\lambda_X(t_1), \lambda_X(t_2)) &= \inf \left\{ \tilde{G}d(t') \mid t' \in \Gamma_G(\lambda_X(t_1), \lambda_X(t_2)) \right\} \\ &\leq \inf \left\{ \tilde{G}d(\lambda_{X \times X}(t)) \mid t \in \Gamma_F(t_1, t_2) \right\} \\ &\leq \inf \left\{ \tilde{F}d(t) \mid t \in \Gamma_F(t_1, t_2) \right\} = d^{\downarrow F}(t_1, t_2). \end{aligned}$$

4. Using the previous two results and the fact that Wasserstein is an upper bound yields:

$$d^{\uparrow F} = d^{\uparrow G} \circ (\lambda_X \times \lambda_X) \leq d^{\downarrow G} \circ (\lambda_X \times \lambda_X) \leq d^{\downarrow F}$$

and since $d^{\uparrow F} = d^{\downarrow F}$ all these inequalities are equalities. \square

In the remainder of this chapter we will call a natural transformation λ nonexpansive [an isometry] if (and only if) each of its components are nonexpansive [isometries] and write $\bar{\lambda}$ for the resulting natural transformation from \bar{F} to \bar{G} . Instead of checking nonexpansiveness separately for each component of a natural transformation, we can just check the above (in-)equalities involving the two evaluation functions.

By applying these conditions on the unit and multiplication of a given monad, we can now provide sufficient criteria for a monad lifting.

Corollary 5.7.2 (Lifting of a Monad) Let (T, η, μ) be a Set-monad and ev_T an evaluation function for T . Then the following holds.

1. If $ev_T \circ \eta_{[0, T]} \leq id_{[0, T]}$ then η is nonexpansive for both liftings. Hence we obtain the unit $\bar{\eta}: \bar{Id} \Rightarrow \bar{T}$ in PMet.
2. If $ev_T \circ \eta_{[0, T]} = id_{[0, T]}$ then η is an isometry for both liftings.
3. Let $d^T \in \{d^{\uparrow T}, d^{\downarrow T}\}$. If $ev_T \circ \mu_{[0, T]} \leq ev_T \circ T ev_T$ and compositionality holds for TT , i.e., $(d^T)^T = d^{TT}$, then μ is nonexpansive, i.e., $d^T \circ (\mu_X \times \mu_X) \leq (d^T)^T$. This yields the multiplication $\bar{\mu}: \bar{T} \bar{T} \Rightarrow \bar{T}$ in PMet.

Proof. This is an immediate consequence of Theorem 5.7.1. For the unit take $F = Id$ with evaluation function $ev_F = id_{[0, T]}$, hence $d^{\uparrow F} = d^{\downarrow F} = d$ and $G = T$, $ev_G = ev_T$, $\lambda = \eta: Id \Rightarrow T$. For the multiplication take $F = TT$, $G = T$, $ev_F = ev_{TT} = ev_T \circ T ev_T$, $ev_G = ev_T$ and $\lambda = \mu$. \square

We conclude this section with two examples of liftable monads.

Example 5.7.3 (Lifting of the Finite Powerset Monad) We recall from Example 2.3.35 that the finite powerset functor \mathcal{P}_f is part of a monad with unit η consisting of the functions $\eta_X: X \rightarrow \mathcal{P}_f X$, $\eta_X(x) = \{x\}$ and multiplication given by $\mu_X: \mathcal{P}_f \mathcal{P}_f X \rightarrow \mathcal{P}_f X$, $\mu_X(S) = \cup S$. We check if our conditions for the Wasserstein lifting are satisfied. Given $r \in [0, \infty]$ we have $ev_T \circ \eta_{[0, \infty]}(r) = \max\{r\} = r$ and for $S \in \mathcal{P}_f(\mathcal{P}_f[0, T])$ we have $ev_T \circ \mu_{[0, 1]}(S) = \max \cup S = \max \cup_{S \in S} S$ and $ev_T \circ T ev_T(S) = \max(ev_T[S]) = \max\{\max S \mid S \in S\}$ and thus it is easy to see that both values coincide. Moreover, we recall from Example 5.6.8 that we have

compositionality for $\mathcal{P}_f \mathcal{P}_f$. Therefore, by Corollary 5.7.2 η is an isometry and μ nonexpansive.

Example 5.7.4 (Lifting of the Distribution Monad With Finite Support) We recall from Example 2.3.36 (page 44) that the probability distribution functor \mathcal{D}_f is part of a monad: the unit η consists of the functions $\eta_X: X \rightarrow \mathcal{D}_f X$, $\eta_X(x) = \delta_x^X$ where δ_x^X is the Dirac distribution and the multiplication is given by $\mu_X: \mathcal{D}_f \mathcal{D}_f X \rightarrow \mathcal{D}_f X$, $\mu_X(P) = \lambda x. \sum_{q \in \mathcal{D}_f X} P(q) \cdot q(x)$. We consider its Wasserstein lifting. Since $[0, 1] = \mathcal{D}_f 2$ we can see that $ev_{\mathcal{D}_f} = \mu_2$. Using this and the monad laws we have $ev_{\mathcal{D}_f} \circ \eta_{[0,1]} = \mu_2 \circ \eta_{\mathcal{D}_f 2} = id_{\mathcal{D}_f X} = id_{[0,1]}$ and also $ev_{\mathcal{D}_f} \circ \mu_{[0,1]} = \mu_2 \circ \mu_{\mathcal{D}_f 2} = \mu_2 \circ \mathcal{D}_f \mu_2 = ev_{\mathcal{D}_f} \circ \mathcal{D}_f ev_{\mathcal{D}_f}$. Moreover, since we always have optimal couplings, we have compositionality for $\mathcal{D}_f \mathcal{D}_f$ by Theorem 5.6.6. Thus by Corollary 5.7.2 η is an isometry and μ nonexpansive.

5.8 Trace Pseudometrics

Combining all our previous results we now want to use the generalized powerset construction (see Section 2.4.3, page 60) on \mathbf{PMet} instead of \mathbf{Set} to obtain trace pseudometrics. The basic setup is summarized in the (non-commutative) diagram in Figure 5.8.1. We quickly recall that in the usual, qualitative setting

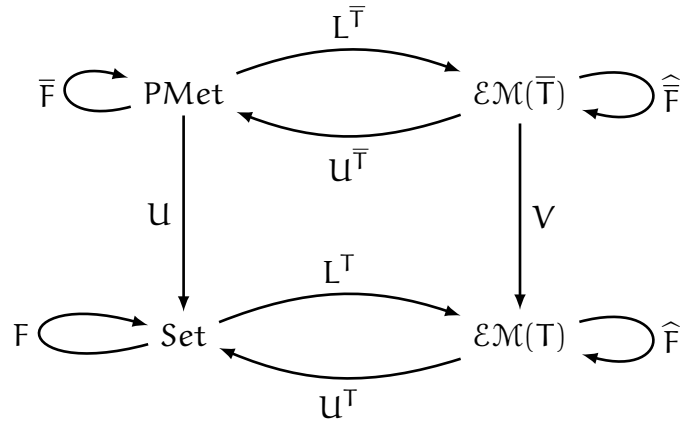


Figure 5.8.1: Trace pseudometrics via the generalized powerset construction

(bottom part of Figure 5.8.1) we have to start with a coalgebra $c: X \rightarrow FTX$ where F is an endofunctor with final coalgebra $z: Z \rightarrow FZ$ and (T, η, μ) is a monad on \mathbf{Set} . Using an \mathcal{EM} -law $\lambda: TF \Rightarrow FT$ we can then consider the determinization $c^\#$ of c which is defined as

$$c^\sharp := \left(TX \xrightarrow{Tc} TFTX \xrightarrow{\lambda_{TX}} FTTX \xrightarrow{F\mu_X} FTX \right).$$

With this determinized coalgebra we define two states $x, y \in X$ of the original coalgebra c to be trace equivalent if and only if $\llbracket \eta_X(x) \rrbracket_c = \llbracket \eta_X(y) \rrbracket_c$ holds.

The underlying reason why this technique works is that the \mathcal{EM} -law λ yields a unique lifting (with respect to the canonical adjunction $L^T \dashv U^T$, see Theorem 2.3.44 on page 47) of the functor F to a functor \widehat{F} on the Eilenberg-Moore category $\mathcal{EM}(T)$. The determinization of a coalgebra is nothing but the application of another lifting

$$L: \text{CoAlg}(FT) \rightarrow \text{CoAlg}(\widehat{F})$$

of the free algebra functor L^T , i.e., $c^\sharp = U^T L(c): TX \rightarrow FTX$ is the F -coalgebra underlying the \widehat{F} -coalgebra $L(c): \mu_X \rightarrow \widehat{F}\mu_X$.

In order to move to a quantitative setting (upper part of Figure 5.8.1) we need to require that both the functor F and the monad (T, η, μ) can be lifted. Then clearly any FT -coalgebra $c: X \rightarrow FTX$ can be regarded as an $\bar{F}\bar{T}$ -coalgebra \bar{c} by equipping the state space X with the discrete metric d assigning \top to non equal states (in this way, \bar{c} is trivially nonexpansive). Moreover, if we can ensure that the \mathcal{EM} law λ is nonexpansive, thus yielding an \mathcal{EM} -law $\bar{\lambda}: \bar{T}\bar{F} \Rightarrow \bar{F}\bar{T}$, we can use exactly the same ideas as before. In particular, we can lift the lifted functor \bar{F} to a functor

$$\widehat{\bar{F}}: \mathcal{EM}(\bar{T}) \rightarrow \mathcal{EM}(\bar{T})$$

on the Eilenberg-Moore category of the lifted monad. With this, we can lift the free algebra functor $L^{\bar{T}}$ to a functor

$$L': \text{CoAlg}(\bar{F}\bar{T}) \rightarrow \text{CoAlg}(\widehat{\bar{F}})$$

which allows us to determinize \bar{c} (as $\bar{F}\bar{T}$ -coalgebra in PMet) to the $\widehat{\bar{F}}$ -coalgebra $L'\bar{c}: \bar{\mu}_X \rightarrow \widehat{\bar{F}}\bar{\mu}_X$ which is given by the underlying \bar{F} -coalgebra

$$\bar{c}^\sharp := U^T L'\bar{c} = \bar{F}\bar{\mu}_X \circ \bar{\lambda}_{TX} \circ \bar{T}\bar{c}: \bar{T}(X, d) \rightarrow \bar{F}\bar{T}(X, d). \quad (5.8.1)$$

If we now equip TX with the behavioral pseudometric $\text{bd}_{c^\sharp}: (TX)^2 \rightarrow [0, \top]$ as in Definition 5.5.4, we can define the trace pseudometric on X via the unit η as follows.

Definition 5.8.1 (Trace Pseudometric) Let F be an endofunctor and (T, η, μ) be a monad on Set . If

1. F has a final coalgebra $z: Z \rightarrow FZ$ in Set ,
2. F has a lifting $\bar{F}: \text{PMet} \rightarrow \text{PMet}$,
3. (T, η, μ) has a lifting $(\bar{T}, \bar{\eta}, \bar{\mu})$, and
4. there is an \mathcal{EM} -law $\lambda: TF \rightarrow FT$ which can be lifted to an \mathcal{EM} -law $\bar{\lambda}: \bar{T}\bar{F} \rightarrow \bar{F}\bar{T}$ then for any coalgebra $c: X \rightarrow FTX$ we define the *trace pseudometric* to be

$$\text{td}_c := \text{bd}_{c^\sharp} \circ (\eta_X \times \eta_X): X \times X \rightarrow [0, \top]$$

where $c^\sharp = F\mu_X \circ \lambda_{TX} \circ Tc: TX \rightarrow FTX$ is the determinization of the coalgebra $c: X \rightarrow FTX$ and $\text{bd}_{c^\sharp}: (TX)^2 \rightarrow [0, \top]$ is the corresponding bisimilarity pseudometric as in Definition 5.5.4 (page 187).

In order to apply this definition to our two main examples (nondeterministic and probabilistic automata) the only missing thing is the lifting of the \mathcal{EM} -law to PMet . We note that Theorem 5.7.1 (page 206) not only provides sufficient conditions for monad liftings but also can be exploited to lift distributive laws. The additional commutativity requirements for \mathcal{KL} -laws or \mathcal{EM} -laws trivially hold when all components are nonexpansive. For the Wasserstein lifting it suffices to require compositionality on the left hand side of the law and to check one inequality.

Corollary 5.8.2 (Lifting of a Distributive Law) Let F, G be weak pullback preserving endofunctors on Set with well-behaved evaluation functions ev_F, ev_G and $\lambda: FG \Rightarrow GF$ be a distributive law. If the evaluation functions satisfy $(\text{ev}_G * \text{ev}_F) \circ \lambda_{[0, \top]} \leq \text{ev}_F * \text{ev}_G$ and compositionality holds for FG , then λ is nonexpansive for the Wasserstein lifting and hence $\bar{\lambda}: \bar{F}\bar{G} \Rightarrow \bar{G}\bar{F}$ is also a distributive law.

Proof. We use the evaluation function $\text{ev}_F * \text{ev}_G$ for FG and for GF the evaluation function $\text{ev}_G * \text{ev}_F$. By Theorem 5.7.1 (page 206) we know that $d^{\downarrow GF} \circ (\lambda_X \times \lambda_X) \leq d^{\downarrow FG}$ and by Lemma 5.6.5.2 (page 197) we have $(d^{\downarrow F})^{\downarrow G} \leq d^{\downarrow GF}$. Plugging everything together we conclude that for every pseudometric space (X, d) we have

$$(d^{\downarrow F})^{\downarrow G} \circ (\lambda_X \times \lambda_X) \leq d^{\downarrow GF} \circ (\lambda_X \times \lambda_X) \leq d^{\downarrow FG} = (d^{\downarrow G})^{\downarrow F}$$

which is the desired nonexpansiveness of λ_X . □

In the remainder of this section we will consider two examples where in both cases G is the machine endofunctor $M_B = B \times _{}^A$ of Example 2.4.5 (for $B = 2$ and $B = [0, 1]$). We recall from Example 2.4.10 that for every output set B the final coalgebra for M_B is

$$z = \langle o_z, s_z \rangle: B^{A^*} \rightarrow B \times (B^{A^*})^A$$

which maps any function $f: A^* \rightarrow B$ to the tuple $z(f) = (o_z(f), s_z(f))$. The output value $o_z(f)$ is the value of f on the empty word, i.e., $o_z(f) = f(\varepsilon)$ and the successor function $s_z(f): A \rightarrow B^{A^*}$ assigns to each letter $a \in A$ the function $s_z(f)(a): A^* \rightarrow B$. Its value on a word $w \in A^*$ is equal to the value of f on the word aw , formally $s_z(f)(a)(w) = f(aw)$. In order to lift the machine functor we have two possibilities:

1. We can lift it as an endofunctor obtaining an endofunctor \overline{M}_B on PMet .
2. We lift the machine bifunctor M of Example 5.6.10 to obtain a lifted bifunctor $\overline{M}: \text{PMet}^2 \rightarrow \text{PMet}$. Then we fix a pseudometric d_B on the outputs B and consider the induced endofunctor $\overline{M}_{(B, d_B)} := \overline{M}((B, d_B), _)$.

In the first case we can of course simply apply Corollary 5.8.2 from above but in the second case we have to prove nonexpansiveness of λ separately. We will employ the first approach for nondeterministic automata (where $B = 2$) and the second one for probabilistic automata (where $B = [0, 1]$).

5.8.1 Trace Pseudometric for Nondeterministic Automata

We will now consider the \mathcal{EM} -law $\lambda: \mathcal{P}_f M_2 \Rightarrow M_2 \mathcal{P}_f$ for finitely branching nondeterministic automata which we have already discussed in Definition 2.4.19 (page 62). Here, Corollary 5.8.2 is directly applicable using $F = \mathcal{P}_f$ and $G = M_2 = 2 \times _{}^A$.

Lemma 5.8.3 (\mathcal{EM} -law for Nondeterministic Automata) Let $(\mathcal{P}_f, \eta, \mu)$ be the finite powerset monad from Example 5.7.3 with the maximum as evaluation function and $M_2 = 2 \times _{}^A$ be the deterministic automaton function equipped with the evaluation function $ev_{M_2}: 2 \times [0, \top]^A \rightarrow [0, \top]$, $ev_{M_2}(o, s) = c \cdot \max_{a \in A} s(a)$ with $c \in]0, 1]$ as in Example 5.6.11. We consider the \mathcal{EM} -law $\lambda: \mathcal{P}_f(2 \times _{}^A) \Rightarrow 2 \times \mathcal{P}_f(_{}^A)$ on Set which is defined, for any set X , as $\lambda_X(S) = \langle o, s \rangle$ with $o(S) = 1$ if there is an $s' \in X^A$ such that $(1, s') \in S$ else $o(S) = 0$ and the successor functions

$$s(S): A \rightarrow \mathcal{P}X, \quad s(A) = \{s'(a) \mid (o', s') \in S\}$$

for every $S \in \mathcal{P}(2 \times X^A)$ as presented in Definition 2.4.19 (page 62). This law is nonexpansive.

Proof. In the notation of Corollary 5.8.2 we have $F = 2 \times _^A = M_2$, and $G = \mathcal{P}_f$. The composed evaluation functions are $ev_{\mathcal{P}_f} * ev_{M_2}: \mathcal{P}_f(2 \times [0, 1]^A) \rightarrow [0, 1]$ where for $S \in \mathcal{P}_f(2 \times [0, 1]^A)$

$$\begin{aligned} ev_{\mathcal{P}_f} * ev_{M_2}(S) &= ev_{\mathcal{P}_f} \circ \mathcal{P}_f ev_{M_2}(S) = \max\{ev_{M_2}(o, s) \mid (o, s) \in S\} \\ &= \max\left\{c \cdot \max_{a \in A} s(a) \mid (o, s) \in S\right\} = c \cdot \max_{(o, s) \in S} \max_{a \in A} s(a) \end{aligned}$$

and $ev_{M_2} * ev_{\mathcal{P}_f}: 2 \times (\mathcal{P}_f[0, 1])^A \rightarrow [0, 1]$ where for $(o, s) \in 2 \times (\mathcal{P}_f X)^A$

$$\begin{aligned} ev_{M_2} * ev_{\mathcal{P}_f}(S) &= ev_{M_2} \circ M_2 ev_{\mathcal{P}_f}(o, s) \\ &= ev_{M_2}(o, \max \circ s) = c \cdot \max_{a \in A} \max s(a) \end{aligned}$$

As we have seen in Example 5.6.9 (page 200) we have compositionality for $\mathcal{P}_f M_2$ and the Wasserstein lifting. We want to apply Corollary 5.8.2 to show nonexpansiveness. For this we just have to check that $(ev_{\mathcal{P}_f} * ev_{M_2}) \circ \lambda_{[0, 1]} \leq ev_{M_2} * ev_{\mathcal{P}_f}$ holds. Indeed we have, for $S \in \mathcal{P}_f(2 \times [0, 1]^A)$,

$$\begin{aligned} (ev_{\mathcal{P}_f} * ev_{M_2}) \circ \lambda_{[0, 1]}(S) &= c \cdot \max_{a \in A} \max\{s(a) \mid (o, s) \in S\} \\ &= c \cdot \max_{a \in A} \max_{(o, s) \in S} s(a) = ev_{M_2} * ev_{\mathcal{P}_f}(S) \end{aligned}$$

which concludes the proof. \square

With this result at hand we can now define the trace pseudometric for finitely branching nondeterministic automata.

Example 5.8.4 (Trace Pseudometric for Nondeterministic Automata) We consider the machine endofunctor $M_2 = 2 \times _^A$. As maximal distance we take $\top = 1$ and as evaluation function we use $ev_{M_2}: [0, 1] \times [0, 1]^A$ with $ev_{M_2}(o, s) = c \cdot \max_{a \in A} s(a)$ for $0 < c < 1$ as in Example 5.5.2 (page 185) and lift the functor using the Wasserstein lifting.

We now take a finitely branching nondeterministic automaton which is a coalgebra $\alpha: X \rightarrow 2 \times (\mathcal{P}_f X)^A$. Its determinization is the powerset automaton $\alpha^\sharp: \mathcal{P}_f X \rightarrow 2 \times (\mathcal{P}_f X)^A$ whose states are sets of states of the original automaton. We recall from Example 5.5.5 (page 187) that the bisimilarity pseudometric is the function

$$bd_{\alpha^\sharp}: \mathcal{P}_f X \times \mathcal{P}_f X \rightarrow [0, 1], \quad bd_{\alpha^\sharp}(S, T) = c^{\inf\{n \in \mathbb{N} \mid \exists w \in A^n. [S]_{\alpha^\sharp}(w) \neq [T]_{\alpha^\sharp}(w)\}}.$$

If we apply the construction of Definition 5.8.1 using the unit $\eta_X(x) = \{x\}$ of the powerset monad we obtain the trace pseudometric

$$\text{td}_\alpha: X \times X \rightarrow [0, 1], \quad \text{td}_\alpha(x, y) = c^{\inf\{n \in \mathbb{N} \mid \exists w \in A^n. \llbracket \{x\} \rrbracket_{\alpha^\#}(w) \neq \llbracket \{y\} \rrbracket_{\alpha^\#}(w)\}}.$$

Thus the trace distance of states x and y of α is given by a word w of minimal length which is

- ▷ contained in the language of the state $\{x\}$ of the determinization $\alpha^\#$ and
- ▷ *not* contained in the language of the state $\{y\}$ of the determinization $\alpha^\#$.

Then, the distance is computed as $c^{|w|}$.

5.8.2 Trace Pseudometric for Probabilistic Automata

Our next example of an \mathcal{EM} -law will be of the shape $\lambda: \mathcal{D}_f M_{[0,1]} \rightarrow M_{[0,1]} \mathcal{D}_f$. This is much more complicated because we need to consider multifunctors to obtain the correct lifting.

Lemma 5.8.5 (\mathcal{EM} -law for Probabilistic Automata) Let $(\mathcal{D}_f, \eta, \mu)$ be the distribution monad with finite support from Example 5.7.4 (page 209) and M be the machine bifunctor from Example 5.6.10 (page 203). There is a known¹⁵ \mathcal{EM} -law $\lambda: \mathcal{D}_f([0, 1] \times _^\mathbb{A}) \Rightarrow [0, 1] \times \mathcal{D}_f^\mathbb{A}$ in **Set** where $\lambda_X = \langle o_X, s_X \rangle$ with

$$\begin{aligned} o_X(P) &= \sum_{r \in [0,1]} r \cdot P(r, X^\mathbb{A}) \\ s_X(P): A \rightarrow \mathcal{D}_f X, \quad s_X(P)(a)(x) &= \sum_{s' \in X^\mathbb{A}, s'(a)=x} P([0, 1], s') \end{aligned}$$

for all sets X and all distributions $P: [0, 1] \times X^\mathbb{A} \rightarrow [0, 1]$. The endofunctors on both sides of this law can be seen as bifunctors F, G for which one component is fixed. They arise by composition of the distribution functor, the identity functor and the machine bifunctor as follows. The bifunctor on the left hand side (the domain of λ) is $F = \mathcal{D}_f \circ M$ and the bifunctor on the right hand side (the codomain of λ) is $G = M \circ (\text{Id} \times \mathcal{D}_f)$ and to get our law we need to fix the respective first parameter to be $[0, 1]$.

If we use the usual evaluation function for the distribution functor as given in Examples 5.4.9 and 5.4.30 (pages 149 and 164), the identity function as evaluation function for Id and the discounted sum for the machine bifunctor as in

¹⁵This law arises out of the so-called *strength map* of the monad [JSS15, Lemma 4]. Since we have not discussed this map in this thesis, we have included an elementary proof in Appendix A.3 using only the definition of an \mathcal{EM} -law.

Example 5.6.10 (page 203), lift both bifunctors and then fix their first component to the metric space $([0, 1], d_e)$ then the above \mathcal{EM} -law is nonexpansive.

Proof. Since all of the involved (bi)functors have optimal couplings, we have compositionality and the evaluation functions for the composed functors are

$$\begin{aligned} ev_F &:= ev_{\mathcal{D}_f} \circ \mathcal{D}_f ev_M: \mathcal{D}_f([0, 1] \times [0, 1]^A) \rightarrow [0, 1] \quad \text{and} \\ ev_G &:= ev_M \circ M(id_{[0, 1]}, ev_{\mathcal{D}_f}): [0, 1] \times (\mathcal{D}_f X)^A \rightarrow [0, 1]. \end{aligned}$$

We will now assume (and prove below) that there exists a function

$$\Lambda_X: \mathcal{D}_f([0, 1]^2 \times (X \times X)^A) \rightarrow [0, 1]^2 \times (\mathcal{D}_f(X \times X))^A$$

which transfers F-couplings to suitable G-couplings in the following sense. For any $P_1, P_2 \in \mathcal{D}_f([0, 1] \times X^A)$ and any $P \in \Gamma_F(P_1, P_2) \subseteq \mathcal{D}_f([0, 1] \times [0, 1] \times (X \times X)^A)$ the function Λ_X has to satisfy the following two requirements

$$\Lambda_X(P) \in \Gamma_G(\lambda_X(P_1), \lambda_X(P_2)) \quad (5.8.2)$$

$$\tilde{G}(d_B, d)(\Lambda_X(P)) \leq \tilde{F}(d_B, d)(P) \quad (5.8.3)$$

because then we have

$$\begin{aligned} (d_B, d)^{\downarrow G}(\lambda_X(P_1), \lambda_X(P_2)) &= \inf \left\{ \tilde{G}(d_B, d)(P') \mid P' \in \Gamma_G(\lambda_X(P_1), \lambda_X(P_2)) \right\} \\ &\leq \inf \left\{ \tilde{G}(d_B, d)(\Lambda_X(P)) \mid P \in \Gamma_F(P_1, P_2) \right\} \\ &\leq \inf \left\{ \tilde{F}(d_B, d)(P) \mid P \in \Gamma_F(P_1, P_2) \right\} \\ &= (d_B, d)^{\downarrow F}(P_1, P_2) \end{aligned}$$

which, due to compositionality, proves the desired nonexpansiveness of λ_X . \square

So let us now define the function Λ_X which we need for the previous proof and prove that it satisfies (5.8.2) and (5.8.3).

Definition 5.8.6 For any set X we define the function

$$\Lambda_X := \langle o_1, o_2, s \rangle: \mathcal{D}_f([0, 1]^2 \times (X \times X)^A) \rightarrow [0, 1]^2 \times (\mathcal{D}_f(X \times X))^A$$

where for any $P \in \mathcal{D}_f([0, 1] \times [0, 1] \times (X \times X)^A)$

$$o_1(P) = \sum_{r \in [0, 1]} r \cdot P(r, [0, 1], (X \times X)^A),$$

$$o_2(P) = \sum_{r \in [0, 1]} r \cdot P([0, 1], r, (X \times X)^A), \text{ and}$$

$$s(P): A \rightarrow \mathcal{D}_f(X \times X), \quad s(P)(a)(x, y) = \sum_{s' \in (X \times X)^A, s'(a)=(x, y)} P([0, 1]^2, s')$$

completely analogous to the definition of the components λ_X of the distributive law in Lemma 5.8.5.

Let us now show that the above definition of Λ_X satisfies our requirements.

Lemma 5.8.7 For any $P_1, P_2 \in \mathcal{D}_f([0, 1] \times X^A)$ and any $P \in \Gamma_F(P_1, P_2)$ the function Λ_X satisfies (5.8.2), i.e., we have $\Lambda_X(P) \in \Gamma_G(\lambda_X(P_1), \lambda_X(P_2))$.

Proof. Let $\pi_i: [0, 1]^2 \rightarrow [0, 1]$ and $\tau_i: X^2 \rightarrow X$ be the projections to the i -th component of the binary products. Since $P \in \Gamma_F(P_1, P_2)$ we know $F(\pi_i, \tau_i) = P_i$. In order to show (5.8.2), we have to prove that the equation

$$G(\pi_i, \tau_i)(\Lambda_X(P)) = \lambda_X(P_i) \quad (5.8.4)$$

holds. Let $\lambda_X = \langle o_X, s_X \rangle$ be defined as in Lemma 5.8.5, and o_1, o_2 , and s as in Definition 5.8.6. The left hand side of (5.8.4) evaluates to

$$\begin{aligned} G(\pi_i, \tau_i)(\Lambda_X(P)) &= (\pi_i \times (\mathcal{D}_f \tau_i)^A)(o_1(P), o_2(P), s(P)) \\ &= (o_i(P), \mathcal{D}_f \tau_i \circ s(P)) \end{aligned} \quad (5.8.5)$$

and since $F(\pi_i, \tau_i) = P_i$ the right hand side of (5.8.4) evaluates to

$$\begin{aligned} \lambda_X(P_i) &= \lambda_X(F(\pi_i, \tau_i)(P)) \\ &= \left(o_X(\mathcal{D}_f(\pi_i \times \tau_i^A)(P)), s_X(\mathcal{D}_f(\pi_i \times \tau_i^A)(P)) \right). \end{aligned} \quad (5.8.6)$$

In order to prove (5.8.4) we will thus have to show that the equalities

$$o_X(\mathcal{D}_f(\pi_i \times \tau_i^A)(P)) = o_i(P), \text{ and} \quad (5.8.7)$$

$$s_X(\mathcal{D}_f(\pi_i \times \tau_i^A)(P)) = \mathcal{D}_f \tau_i \circ s(P) \quad (5.8.8)$$

hold. We first check the output values and observe that

$$\begin{aligned} o_X(\mathcal{D}_f(\pi_i \times \tau_i^A)(P)) &= \sum_{r \in [0, 1]} r \cdot \mathcal{D}_f(\pi_i \times \tau_i^A)(P)(r, X^A) \\ &= \sum_{r \in [0, 1]} r \cdot \left(P \circ (\pi_i \times \tau_i^A)^{-1}[\{r\} \times X^A] \right) \\ &= \sum_{r \in [0, 1]} r P \left(\left\{ (o_1, o_2, s') \in \mathcal{D}_f([0, 1]^2 \times (X^2)^A) \mid \pi_i \times \tau_i^A(o_1, o_2, s') \in \{r\} \times X^A \right\} \right) \\ &= \sum_{r \in [0, 1]} r P \left(\left\{ (o_1, o_2, s') \in \mathcal{D}_f([0, 1]^2 \times (X^2)^A) \mid o_i = r \right\} \right) = o_i(P) \end{aligned}$$

showing that indeed (5.8.7) holds. The left hand side of (5.8.8) evaluates to

$$\begin{aligned}
s\left(\mathcal{D}_f(\pi_i \times \tau_i^A)(P)\right)(a)(x) &= \sum_{\{s' \in X^A, s'(a)=x\}} \mathcal{D}_f(\pi_i \times \tau_i^A)(P)([0, 1], s') \\
&= \sum_{s' \in X^A, s'(a)=x} P\left(\left\{(o_1, o_2, s'') \in \mathcal{D}_f([0, 1]^2 \times (X^2)^A) \mid \tau_i \circ s'' = s'\right\}\right) \\
&= \sum_{s'' \in (X \times X)^A, \tau_i \circ s''(a)=x} P([0, 1]^2, s'')
\end{aligned}$$

and the right hand side of (5.8.8) also evaluates to

$$\begin{aligned}
(\mathcal{D}_f \tau_i \circ s(P))(a)(x) &= s(P)(a) \circ \tau_i^{-1}[\{x\}] \\
&= s(P)(a)(\{y \in X \times X \mid \tau_i(y) = x\}) \\
&= \sum_{s'' \in (X \times X)^A, \tau_i \circ s''(a)=x} P([0, 1]^2, s'')
\end{aligned}$$

which shows that equation (5.8.8) holds and thus (5.8.5) and (5.8.6) coincide. Therefore (5.8.4) holds i.e., we have proved $\Lambda_X(P) \in \Gamma_G(\lambda_X(P_1), \lambda_X(P_2))$. \square

Lemma 5.8.8 For any $P_1, P_2 \in \mathcal{D}_f([0, 1] \times X^A)$ and any $P \in \Gamma_F(P_1, P_2)$ the function Λ_X satisfies (5.8.3), i.e., we have $\tilde{G}(d_B, d)(\Lambda_X(P)) \leq \tilde{F}(d_B, d)(P)$.

Proof. Let o_1, o_2 and s be defined as in Definition 5.8.6. The left hand side of (5.8.3) evaluates to

$$\begin{aligned}
\tilde{G}(d_B, d)(\Lambda_X(P)) &= (ev_G \circ G(d_B, d))(\lambda_X(P)) = ev_G\left(G(d_B, d)(\Lambda_X(P))\right) \\
&= ev_G\left((d_B \times (\mathcal{D}_f d)^A)(o_1(P), o_2(P), s(P))\right) \\
&= ev_G\left(d_B(o_1(P), o_2(P)), a \mapsto \mathcal{D}_f d(s(P)(a))\right) \\
&= \left(ev_M \circ M(id_{[0, 1]}, ev_{\mathcal{D}_f})\right)\left(d_B(o_1(P), o_2(P)), a \mapsto \mathcal{D}_f d(s(P)(a))\right) \\
&= ev_M\left(M(id_{[0, 1]}, ev_{\mathcal{D}_f})\left(d_B(o_1(P), o_2(P)), a \mapsto \mathcal{D}_f d(s(P)(a))\right)\right) \\
&= ev_M\left(d_B(o_1(P), o_2(P)), ev_{\mathcal{D}_f}^A(a \mapsto \mathcal{D}_f d(s(P)(a)))\right) \\
&= ev_M\left(d_B(o_1(P), o_2(P)), a \mapsto ev_{\mathcal{D}_f}(\mathcal{D}_f d(s(P)(a)))\right) \\
&= c_1 d_B(o_1(P), o_2(P)) + \frac{c_2}{|A|} \sum_{a \in A} ev_{\mathcal{D}_f}(\mathcal{D}_f d(s(P)(a))) \tag{5.8.9}
\end{aligned}$$

and since for each $\alpha \in A$ we have

$$\begin{aligned} \text{ev}_{\mathcal{D}_f}(\mathcal{D}_f d(\mathfrak{s}(P)(\alpha))) &= \sum_{r \in [0,1]} r \cdot \mathfrak{s}(P)(\alpha)(d^{-1}[\{r\}]) = \sum_{(x,y) \in X^2} d(x,y) \cdot \mathfrak{s}(P)(\alpha)(x,y) \\ &= \sum_{(x,y) \in X^2} d(x,y) \cdot \left(\sum_{s' \in (X \times X)^A, s'(\alpha) = (x,y)} P([0,1]^2, s') \right) \\ &= \sum_{s' \in (X \times X)^A} d(s'(\alpha)) \cdot P([0,1]^2, s') \end{aligned}$$

we may continue (5.8.9) as follows:

$$\begin{aligned} \tilde{G}(d_B, d)(\Lambda_X(P)) \\ = c_1 d_B(o_1(P), o_2(P)) + \frac{c_2}{|A|} \sum_{\alpha \in A} \sum_{s' \in (X \times X)^A} d(s'(\alpha)) \cdot P([0,1]^2, s'). \end{aligned} \quad (5.8.10)$$

For the right hand side of (5.8.3) we have

$$\begin{aligned} \tilde{F}(d_B, d)(P) &= (\text{ev}_F \circ F(d_B, d))(P) = \left((\text{ev}_{\mathcal{D}_f} \circ \mathcal{D}_f \text{ev}_M) \circ \mathcal{D}_f(M(d_B, d)) \right)(P) \\ &= \text{ev}_{\mathcal{D}_f} \left(\mathcal{D}_f \text{ev}_M \left(\mathcal{D}_f(M(d_B, d))(P) \right) \right) = \text{ev}_{\mathcal{D}_f} \left(\mathcal{D}_f \text{ev}_M \left(\mathcal{D}_f(d_B \times d^A)(P) \right) \right) \\ &= \text{ev}_{\mathcal{D}_f} \left(\left(\mathcal{D}_f(d_B \times d^A)(P) \right) \circ \text{ev}_M^{-1} \right) = \sum_{r \in [0,1]} r \cdot \left(\mathcal{D}_f(d_B \times d^A)(P) \right) (\text{ev}_M^{-1}[\{r\}]) \\ &= \sum_{(o,s) \in [0,1] \times [0,1]^A} \text{ev}_M(o, s) \cdot \left(\mathcal{D}_f(d_B \times d^A)(P) \right) (o, s) \\ &= \sum_{(o,s) \in [0,1] \times [0,1]^A} \text{ev}_M(o, s) \cdot P \left((d_B \times d^A)^{-1}[\{(o, s)\}] \right) \\ &= \sum_{(o_1, o_2, s') \in [0,1]^2 \times (X \times X)^A} \text{ev}_M \left((d_B \times d^A)(o_1, o_2, s') \right) \cdot P(o_1, o_2, s') \\ &= \sum_{(o_1, o_2, s') \in [0,1]^2 \times (X \times X)^A} \text{ev}_M \left(d_B(o_1, o_2), \lambda \alpha. d(s'(\alpha)) \right) \cdot P(o_1, o_2, s') \\ &= \sum_{(o_1, o_2, s') \in [0,1]^2 \times (X \times X)^A} \left(c_1 d_B(o_1, o_2) + \frac{c_2}{|A|} \sum_{\alpha \in A} d(s'(\alpha)) \right) \cdot P(o_1, o_2, s') \\ &= c_1 o(P) + \frac{c_2}{|A|} \sum_{s' \in (X \times X)^A} \sum_{\alpha \in A} d(s'(\alpha)) \cdot P([0,1]^2, s') \end{aligned} \quad (5.8.11)$$

with

$$\mathfrak{o}(P) = \sum_{(o_1, o_2) \in [0,1]^2} d_B(o_1, o_2) \cdot P(o_1, o_2, (X \times X)^A).$$

Comparing (5.8.10) and (5.8.11) we see that in order to obtain inequality (5.8.3) we just have to show

$$d_B(\mathfrak{o}_1(P), \mathfrak{o}_2(P)) \leq \mathfrak{o}(P)$$

This is easily done using the fact that $d_B = d_e$ is the Euclidean metric and the triangle inequality:

$$\begin{aligned} d_B(\mathfrak{o}_1(P), \mathfrak{o}_2(P)) &= \\ &= \left| \sum_{r_1 \in [0,1]} r_1 \cdot P(r_1, [0,1], (X \times X)^A) - \sum_{r_2 \in [0,1]} r_2 \cdot P([0,1], r_2, (X \times X)^A) \right| \\ &= \left| \sum_{r_1, r_2 \in [0,1]} r_1 \cdot P(r_1, r_2, (X \times X)^A) - \sum_{r_1, r_2 \in [0,1]} r_2 \cdot P(r_1, r_2, (X \times X)^A) \right| \\ &= \left| \sum_{r_1, r_2 \in [0,1]} (r_1 - r_2) \cdot P(r_1, r_2, (X \times X)^A) \right| \\ &\leq \sum_{r_1, r_2 \in [0,1]} |(r_1 - r_2) \cdot P(r_1, r_2, (X \times X)^A)| \\ &= \sum_{r_1, r_2 \in [0,1]} |r_1 - r_2| \cdot P(r_1, r_2, (X \times X)^A) = \mathfrak{o}(P). \end{aligned}$$

We have thus also completed the proof of the inequality (5.8.3). \square

With these two lemmas we have all the ingredients needed for the proof of Lemma 5.8.5, so we now have a suitable lifting of the distributive law for probabilistic automata.

Example 5.8.9 (Trace Pseudometric for Probabilistic Automata) As in Example 5.6.12 (page 205) we consider the machine functor $M_{[0,1]} = [0,1] \times _^A$ which arises out of the machine bifunctor M by fixing the first component to $[0,1]$. As maximal distance we set $\top = 1$ and equip the machine bifunctor M with the evaluation function $ev_M: [0,1] \times [0,1]^A$ where

$$ev_M(o, s) = c_1 o + c_2 |A|^{-1} \sum_{a \in A} s(a)$$

for $c_1, c_2 \in]0, 1[$ such that $c_1 + c_2 \leq 1$ as in Example 5.6.10. We lift this bifunctor using the Wasserstein lifting and then fix its first component to $([0, 1], d_e)$.

For a probabilistic automaton $\alpha: X \rightarrow [0, 1] \rightarrow (\mathcal{D}_f X)^A$ its determinization is the $M_{[0,1]}$ -coalgebra $\alpha^\sharp: \mathcal{D}_f X \rightarrow [0, 1] \rightarrow (\mathcal{D}_f X)^A$ whose state space are distributions on the states of the original automaton. From Example 5.6.12 we know that we obtain the following bisimilarity pseudometric

$$\text{bd}_{\alpha^\sharp}: \mathcal{D}_f X \times \mathcal{D}_f X \rightarrow [0, 1], \quad \text{bd}_{\alpha^\sharp}(p, q) = c_1 \cdot \sum_{w \in A^*} \left(\frac{c_2}{|A|} \right)^{|w|} |\llbracket p \rrbracket_{\alpha^\sharp}(w) - \llbracket q \rrbracket_{\alpha^\sharp}(w)|$$

If we apply the construction of Definition 5.8.1 using the unit $\eta_X(x) = \delta_x^X$ of the finite distribution monad we obtain the trace pseudometric

$$\text{td}_\alpha: X \times X \rightarrow [0, 1], \quad \text{td}_\alpha(x, y) = c_1 \cdot \sum_{w \in A^*} \left(\frac{c_2}{|A|} \right)^{|w|} \left| \llbracket \delta_x^X \rrbracket_{\alpha^\sharp}(w) - \llbracket \delta_y^X \rrbracket_{\alpha^\sharp}(w) \right|.$$

Thus the trace distance of states x and y of α is given by the distance of their Dirac distributions in the determinization.

5.9 Conclusion, Related and Future Work

In this final main chapter we have seen how a lot of the coalgebraic machinery for modelling and analyzing labelled transition systems can be extended from a qualitative to a quantitative setting. The crucial idea for this is the idea to lift a functor from the category **Set** of sets and functions to the category **PMet** of pseudometric spaces and nonexpansive functions. While all the remaining results require a bit of effort, they arise naturally once such lifting has been defined. The big advantage of our approach is that we try

- ▷ to keep it as general as possible (by using coalgebra and not restricting to a specific class of transition systems) and
- ▷ to minimize the amount of additional information needed.

Instead of assuming that a transition system already comes equipped with some distance function on the state space, we give canonical definitions of bisimilarity and trace pseudometrics in the sense that they arise automatically out of the coalgebraic model. The only information we have to provide is the evaluation function which explains how we can evaluate the effect of applying the branching functor to real numbers as a single real number.

Whenever someone is interested in defining a new type of transition system, he can now automatically derive canonical notions of both behavioral equivalences and pseudometrics.

5.9.1 Related Work

The ideas for our framework are not only heavily influenced by transportation theory [Vil09] but also by work on quantitative variants of (bisimulation) equivalence of probabilistic systems. In that context Alessandro Giacalone, Chi-Chang Jou and Scott A. Smolka observed in the nineties that probabilistic Larsen-Skou bisimulation [LS89] is too strong and therefore introduced a metric based on the notion of ε -bisimulations [GJS90]. Such a bisimulation is a relaxation of the usual probabilistic bisimulation relation which allows matching the steps of another state not with exactly the same probability but with a probability that is at most ε apart with respect to the Euclidean metric on $[0, 1]$. Based on this, two states are exactly ε apart if this is the smallest value such that the two states are ε -bisimilar.

A second approach to behavioral distances is based on logics. Labelled Markov processes (LMP) are generalizations of reactive probabilistic transition system to fairly arbitrary (namely analytic) state spaces which involve some measure theoretic results. Surprisingly, probabilistic bisimilarity for these systems can be expressed via a simple modal logic without negation [DEP98] in the sense that two states of an LMP are bisimilar if and only if they satisfy the same formulae. Using this logical framework Josée Desharnais, Vineet Gupta, Radha Jagadeesan and Prakash Panangaden defined a family of metrics between LMPs [DGJP04] via functional expressions, which can be understood as quantitative generalization of the logical formulae. If evaluated on a state of an LMP, such a functional expression measures the extent (as real number between 0 and 1) to which a formula is satisfied in that state. Then, for any set of such functional expressions, the distance of two LMPs is the supremum of all differences (wrt. to the Euclidean distance on $[0, 1]$) of these functional expressions.

A third, coalgebraic approach, which inspired us to develop our framework, is used by Franck van Breugel and James Worrell [vBW05; vBW06]. As we have presented in the examples in this chapter, they define both a discounted and an undiscounted pseudometric on probabilistic systems via a fixed point approach using the usual Kantorovich pseudometric for probability measures. Moreover, they show that this metric is related to the logical pseudometric by Desharnais et al. [vBW05]. We quickly point out that metrics in a coalgebraic setting appeared already earlier in a paper by Erik de Vink and Jan Rutten. They used ultrametrics¹⁶ and the category of ultrametric spaces in order to define coalgebraic bisimulation for continuous probabilistic transition systems [dVR97;

¹⁶An ultrametric is a reflexive and symmetric function $d: X^2 \rightarrow [0, 1]$ satisfying the implication $d(x, y) \implies x = y$ and the strong triangle inequality $d(x, z) \leq \max\{d(x, y), d(y, z)\}$.

dVR99]. However, they use it mainly as a technical tool to get a final coalgebra and not in order to study bisimilarity distances between these systems.

Not only the definition of distances for probabilistic systems and the study of their theoretical importance but also their efficient approximation or exact computation has been the focus of several recent research papers [vBW01a; FPP04; TDZ11; CPP12]. In particular, Di Chen, Franck van Breugel and James Worrell proved that both the discounted and the undiscounted bisimilarity pseudometric for probabilistic systems can be computed exactly in polynomial time exploiting algorithms to solve linear programs [CvBW12]. Taking some inspiration from this work, one year later Giorgio Bacci, Giovanni Bacci, Kim Larsen and Radu Mardare proposed an on-the-fly approach for the exact computation of bisimilarity distances [BBLM13] which they proved to be practically much more efficient than the earlier approximation algorithms.

Behavioral distances have not only been studied for probabilistic systems but also for other types of transition systems. One apparent example which also appears in the main text is the branching distance for metric transition systems [dAFS09]. Moreover, a thorough comparison of various different behavioral distances on labelled transition systems has recently been carried out by Uli Fahrenberg, Axel Legay and Claus Thrane. They transfer Rob van Glabbeek's quantitative linear-time-branching time spectrum [vGla90] to a quantitative setting [FLT11; FL14].

Finally we remark that there has also been a previous effort to provide a uniform and general framework for behavioral metrics which is, however, not based on coalgebra. In 2006 Yuxin Deng, Tom Chothia, Catuscia Palamidessi and Jun Pang defined action-labelled quantitative transition systems and a theory of state-pseudometrics based on the Kantorovich and Wasserstein metrics for probabilistic systems [DCPP06]. In particular, their largest state-pseudometric (with respect to the reversed pointwise order of pseudometrics) corresponds to bisimilarity and – as in our framework – it can be defined as greatest fixed point of a monotone function (we use the pointwise order of pseudometrics so we take the least fixed point).

5.9.2 Future Work

This chapter proposes a paradigmatic shift from qualitative to quantitative behavior analysis and although many basic results are in place there is still a lot of work ahead. We will first discuss a few open questions whose answers (if they exist) might yield improvements of our current framework. Then we discuss further possible generalizations.

In light of the fact that we propose two different lifting approaches, the

first apparent question is whether there are conditions that guarantee that these liftings coincide, i.e., such that the Kantorovich-Rubinstein duality holds. However, some preliminary attempts to do so suggest that this is very difficult. The proof for the duality in the (arbitrary) probabilistic setting is domain specific and cannot easily be generalized.

Another valid question concerning the two different liftings is whether they can be captured by some *universal properties*. Although we use a coalgebraic and thus category theoretic framework, our intuition comes from transportation and probability theory. It would be interesting to figure out whether there is some general category theoretic construction such that our liftings are two ends of this construction in a similar way as the Kleisli and Eilenberg-Moore categories of a monad are initial and final objects in a category of adjunctions. A possible source of inspiration for this line of work could be Franck van Breugel's draft paper on the metric monad [vBre05] which describes a generalization of the (continuous) Giry monad in terms of universal properties involving monad morphisms.

In order to obtain trace pseudometrics we chose to employ the generalized powerset construction by Alexandra Silva, Filippo Bonchi, Marcello Bonsangue and Jan Rutten [SBBR13], one of the two most prominent coalgebraic approaches to traces. As we have discussed in the Preliminaries (Chapter 2), the other well-known approach is to work in the Kleisli category as suggested by Ichiro Hasuo, Bart Jacobs and Ana Sokolova [HJS07]. An open question that remains is, whether our framework can also be modified or extended to work in that setting. A possible basis for answering this could be the recent comparison between these two approaches in the qualitative setting which was carried out by Bart Jacobs, Alexandra Silva and Ana Sokolova [JSS15]. However, since this is already quite complicated in the qualitative case, it is very likely even more involved to adapt it to the quantitative case. In particular, for this comparison one needs – in addition to the \mathcal{EM} -law – a \mathcal{Kl} -law and a so-called extension natural transformation which connects the two distributive laws.

While our theory is already at a quite general level, there are several further possible generalizations. Among these, one could be to drop symmetry and study so-called *directed pseudometrics* as is done in the case of metric transition systems [dAFS09]. This would lay the foundation to study simulation distances from a coalgebraic perspective.

An even more general idea is to study certain reflexive functions $d: X^2 \rightarrow L$ as generalized metrics, where L is a (complete) lattice with possibly some additional structure. This could result in a theory in which one can model distances for conditional transition systems (CTS). These systems were proposed in 2012 by Jiří Adámek, Filippo Bonchi, Mathias Hülsbusch, Barbara König, Stefan

Milius and Alexandra Silva [ABH+12] and are similar to featured transition systems [CHS+10]. Formally, a CTS is a labelled transition system with the following semantic. Once the environment chooses a label (which represents a condition or a feature), all transitions with this label remain (but the label is dropped) and all the other transitions vanish. Then one is interested in the behavior of the resulting unlabelled transition system. If A is the set of conditions, we could take the complete lattice (with respect to the subset ordering) $L = \mathcal{P}A$ as codomain of our generalized metrics. A natural distance of two states x, y could be the set of conditions for which they are not bisimilar. This is a further generalization of a distance recently proposed by Joanne M. Atlee, Uli Fahrenberg and Axel Legay for featured transition systems: their (simulation) distance only counts how many features prevent simulation [AFL15].

A less drastic, yet interesting generalization could result from replacing the Euclidean metric with a different metric which has recently been suggested by Konstantinos Chatzikokolakis, Daniel Gebler, Catuscia Palamidessi and Lili Xu for probabilistic systems [CGPX14]. Our Kantorovich lifting is obviously based on the Euclidean metric and we could simply replace $d_e: [0, \top]^2 \rightarrow [0, \top]$ with a different metric in this definition and study the resulting liftings. However, it is unclear how to proceed for the Wasserstein lifting since the Euclidean metric only plays a role in Condition W2 of the well-behavedness of the respective evaluation function.

The use of so-called up-to techniques [San98] can significantly reduce both memory consumption and running time for equivalence checks between two specific states of a labelled transition system. This was demonstrated recently by Filippo Bonchi and Damien Pous for the equivalence check of nondeterministic finite automata [BP13]. Together with Daniela Petrişan and Jurriaan Rot, they discovered a fibrational basis for these techniques [BPPR14; Rot15]. Based on some preliminary research, we know that our entire framework can be seen from a fibrational perspective as well, leading to yet another generalization. It is our hope that this fibrational view will lead to more general proofs and efficiently computable algorithms, possibly by using the aforementioned up-to techniques.

Another valid question is, if (and how) our techniques can be generalized to other categories than \mathbf{Set} . In order to talk about distances between states it is likely that this will require at least concrete categories.

As we have discussed above, for probabilistic systems it is possible to efficiently compute the lifted distance by using ideas from linear programming. While our framework provides a solid theoretical basis for reasoning about several behavioral distances, its algorithmic applicability as yet is somewhat limited. For this we would need

- ▷ an efficient method to compute the lifted distances, and possibly also
- ▷ an efficient method to automatically derive the fixed point of Theorem 5.5.1.

However, it is most likely that the efficiency of these methods will to a great extent rely on the specific system under consideration.

Last but not least, the coalgebraic theory in Set has benefited a lot from the huge amount of examples. While we have already looked at several examples throughout this chapter, there is yet a lot more examples that should be worked out explicitly. In particular, it would be interesting to see if (and how) we can recover other behavioral distances from the literature.

Conclusion

THE overall aim of this thesis was to continue the analysis of labelled transition systems using coalgebraic methods. Let us now first briefly sum up the main results of the thesis and then discuss how they fit into the broader scientific context. In a nutshell, the main chapters provide us with

- ▷ an interpretation of the role of adjunctions between coalgebras, which shows that several automata transformations (determinization etc.) are just adjoint functors (Chapter 3),
- ▷ a coalgebraic definition of finite and infinite traces for continuous generative probabilistic transition systems (Chapter 4), and finally
- ▷ a coalgebraic framework for deriving behavioral pseudometrics encompassing both branching time (bisimilarity) pseudometrics as well as linear time (trace) pseudometrics (Chapter 5).

All of these results are independent of each other yet they share a common foundation: the idea that coalgebra allows both to *model* transition systems and more importantly that it provides a canonical method to *analyze* their behavior via the notion of final coalgebra. This validates the transformations of coalgebras using right adjoints in Chapter 3 since they preserve limits and thus the behavior of a system. Moreover, the definition of traces for probabilistic systems in Chapter 4 is just an instance of a final coalgebra. Finally, also the whole framework for behavioral pseudometrics developed in Chapter 5 builds upon the interpretation of final coalgebra as behavior: the fixed-point definition of the behavioral pseudometric yields the final coalgebra for the lifted functor in the category of pseudometric spaces.

6.1 From Qualitative to Quantitative Analyses

While all the results we have presented are interesting in their own right, the most important *conceptual contribution* of this work is the move from qualitative

to quantitative behavioral analyses proposed at great length in the last main chapter (Chapter 5). However, before we discuss these quantitative aspects, let us first assess the significance of the other contributions of this thesis.

Our examination of adjunction liftings in the context of coalgebraic automata models (Chapter 3) did not result in deep new theoretical insights but shed some light on the crucial properties of standard determinization constructions on automata, namely that they are lifted left or right adjoints between categories of coalgebras. This observation adds not only to the understanding of the meaning of adjunctions but might also help to find new determinization constructions for other types of transition systems.

The treatment of arbitrary generative probabilistic systems in the category \mathbf{Meas} of measurable spaces and functions which we discussed in Chapter 4 shows several things. First of all, it proves that the basic idea of the Kleisli approach to trace semantics [HJS07] can also successfully be applied to other base categories than \mathbf{Set} (without the correspondence between initial algebra and final coalgebra). Moreover, our main final coalgebra result (Theorem 4.2.27, page 111) exhibits an interesting correlation of the uniqueness of the arrow into the final coalgebra and the unique extension of a σ -finite pre-measure. Finally, with our theory it is possible to analyze not only finite but also infinite linear behavior of generative probabilistic systems which is impossible in \mathbf{Set} even if the system under consideration can be modelled as coalgebra in \mathbf{Set} . Moreover, looking at the infinite behavior also permits to analyze systems without explicit termination resulting in infinite probabilistic traces.

Let us now turn our attention to the quantitative perspective. It is certainly very easy to just *use* coalgebra in a quantitative setting. For example, systems involving any (real) numbers like probabilistic or weighted transition systems are inherently of a quantitative nature and thus any coalgebra which models such a system carries a quantitative meaning. However, usually such systems are modelled as coalgebras in the category \mathbf{Set} which deprives us of the possibility to analyze these quantitative properties using the coalgebraic machinery. In particular, final coalgebras only yield behavioral *equivalences*.

In order to employ coalgebraic reasoning for behavioral *distances*, one has to work in a suitable category where the quantitative information is captured as part of the category itself such as our category \mathbf{PMet} of pseudometric spaces and nonexpansive functions. In this case, things are very simple if we can start with a coalgebra $c: (X, d) \rightarrow G(X, d)$ in \mathbf{PMet} for a functor G on \mathbf{PMet} which has a final coalgebra $z: (Z, d_Z) \rightarrow G(Z, d_Z)$. Then the apparent canonical definition of a behavioral (bisimilarity) distance is

$$\text{bd}_c: X \times X \rightarrow [0, \top], \quad \text{bd}_c(x, x') := d_Z(\llbracket x \rrbracket_c, \llbracket x' \rrbracket_c) \quad (6.1.1)$$

using the unique coalgebra homomorphism into the final coalgebra which is a nonexpansive function $\llbracket \cdot \rrbracket_c: (X, d) \rightarrow (Z, d_Z)$. Apart from being intuitively the correct one, this definition possesses two important properties.

- ▷ First of all it naturally extends coalgebraic behavioral equivalences: two states which are identified in the final coalgebra ($\llbracket x \rrbracket_c = \llbracket x' \rrbracket_c$) necessarily have distance 0.
- ▷ Moreover, it is the smallest distance on X for which we can define a G -coalgebra structure on (X, d) . In fact, since $\llbracket \cdot \rrbracket_c$ has to be nonexpansive (it must be an arrow in \mathbf{PMet}), we have $\text{bd}_c(x, x') = d_Z(\llbracket x \rrbracket_c, \llbracket x' \rrbracket_c) \leq d(x, x')$ for *every* coalgebra $c: (X, d) \rightarrow G(X, d)$. Conversely this means that every coalgebra $c: (X, d) \rightarrow G(X, d)$ proves that the behavioral distance on X is smaller than or equal to d .

The main difficulty with the above setup is that in many cases it is much easier to model a transition system just as a coalgebra $c: X \rightarrow FX$ in \mathbf{Set} than to do so directly in \mathbf{PMet} . When we take into account the above observations, the problem is not to equip the state space X with a suitable distance d to start with because we can always take the discrete distance which assigns distinct states the distance \top . The difficult part is to define a suitable functor on \mathbf{PMet} . While it is usually easy to figure out how the functor transforms the state space X , one also has to specify how the functor transforms a pseudometric d on X to a pseudometric on FX .

This problem is the starting point for the systematic study of functor liftings which forms the basis for the behavioral pseudometric framework of Chapter 5. Given an endofunctor F on \mathbf{Set} we provide two canonical ways, based solely on a simple evaluation function, to extend this to a functor \bar{F} on \mathbf{PMet} which we call a lifting of F . Moreover, in presence of any lifting, a final F -coalgebra induces a final \bar{F} -coalgebra (see Theorem 5.5.1). Thus, in this case we can define bisimilarity distances as in (6.1.1) using $G = \bar{F}$ as functor (Definition 5.5.4).

As final contribution we also show how to extend the generalized powerset construction [SBBR13] to this quantitative setting using liftings: Whenever this construction is applicable to a coalgebra of the shape $c: X \rightarrow FTX$ for an endofunctor F and a monad (T, η, μ) on \mathbf{Set} , we can check if all the respective parts can be lifted to \mathbf{PMet} . Then – as is to be expected – this construction yields a canonical definition of trace distance as detailed in Definition 5.8.1.

Summing up, we have indeed successfully and with many details demonstrated how to use the coalgebraic machinery for a quantitative analysis of transition systems. However, this is still just an initial step and there are yet many interesting discoveries to be made in this quantitative coalgebraic world (see the discussion in Section 5.9, page 220).

6.2 Pros and Cons of the Coalgebraic Perspective

Apparently, the coalgebraic view requires a lot of non-trivial background knowledge which is not immediately related to the respective systems under investigation. The Preliminaries (Chapter 2) of this thesis provide a short introduction to both category theory as well as coalgebra which should be sufficient to understand this thesis and also some of the most important ideas of the coalgebraic machinery. However, they only cover a very small part of the big picture so in order to properly work with transition systems coalgebraically, one has to be prepared to learn about many more abstract concepts.

The benefit of this high level of abstraction provided by the coalgebraic framework is that it allows to identify *fundamental principles*. By properly hiding the specific details of a transition system, one can often discover the crucial properties of a construction. For example, the determinization of non-deterministic automata can be understood in terms of adjunctions and liftings as we have discussed in Chapter 3. Moreover, this idea also forms the basis for the generalized powerset construction [SBBR13] allowing determinization of various coalgebras in *Set* which we extended to pseudometric spaces in Chapter 5. Of course, the whole behavioral pseudometric framework of that chapter is another example for coalgebraic abstraction. The definitions, theorems and algorithms for the behavioral pseudometrics arise quite naturally just out of the coalgebraic theory. Instead of having to think of them for each transition system separately and showing e.g. that one obtains a pseudometric, we now have a generic and uniform framework for (almost) any transition system that can be modelled as *Set*-coalgebra.

Sticking with this example we can, however, also identify a downside of the coalgebraic abstraction. While the final coalgebra construction in *PMet* (see Theorem 5.5.1) is essentially algorithmic, it is not yet implementable since the only termination guarantee we can provide is termination after ω steps (if the functor is ω -continuous). In order to guarantee termination after finitely many steps or at least some measure of convergence of our algorithm we will most likely have to take into account some specific properties of the respective systems under consideration.

To conclude this very brief discussion, coalgebra can be extremely helpful to understand fundamental theoretic principles underlying several constructions and it permits to state and prove several properties without referring to specific details. However, the level of abstraction makes it difficult to learn and sometimes the lack of details even restrains the expressiveness of the results. Thus it is perhaps best to use coalgebra for a general theory where it excels and resort to the more specific details not only in order to get the ideas for expanding this

theory but also in order to strengthen and extend the general results provided by the coalgebraic machinery.

6.3 Related and Future Work

A detailed description of the possible follow-up works on the topics covered in this thesis and also pointers to related literature can be found in the respective parts at the end of the main chapters. Here we will instead concentrate on a more general perspective and evaluate which future research direction seems most promising.

First of all we remark that the immediate extensibility of the results on coalgebraic traces for continuous probabilistic transition systems as given Chapter 4 is limited. This is simply due to the fact that we have just employed the Kleisli approach to trace equivalences [HJS07] to a very specific setting using methods from measure theory. Thus there is not much hope of a generalization to other transition systems. This line of work can thus serve mainly as a proof of the applicability of the Kleisli approach for other, more complicated categories than \mathbf{Set} and also as a reference for some slightly more complicated final coalgebras. However, as we pointed out already at the end of Chapter 4, since we just constructed our final coalgebras manually, it might still be interesting to find generic final coalgebra constructions in the Kleisli category of the Giry monads.

Although the theoretical contribution about adjoint functor lifting in Chapter 3 is encompassed by an earlier, more general 2-categorical result by Claudio Hermida and Bart Jacobs [HJ98], the chapter can still teach us that it is sometimes also useful to work out examples in detail. In fact, the whole *coalgebras-are-transition-systems*-paradigm is of course only validated by the many examples that have been studied in the literature. In our case – besides the different automata constructions we have (re)discovered – this has lead us to the definition of *deterministic join automata* which are just deterministic automata whose state spaces are complete join semilattices and whose transition function respects this structure. They are a natural generalization of the powerset automaton that arises as the determinization of a nondeterministic automaton. In such an automaton, the join of two states (which are sets of states of the original NFA) is just their set-theoretic union.

To put them in context with the literature, we note that from a theoretic point of view, the state spaces of the powerset automata are simply the free Eilenberg-Moore algebras of the powerset monad whereas the state spaces of deterministic join automata are arbitrary ones. Thus, if we look at other monads, we might wonder whether their free algebras are also state spaces of determinizations

of some systems. This is exactly the view taken in the generalized powerset construction [SBBR13; JSS15]. Moreover, the determinization construction itself is yet another instance of lifting adjunctions to coalgebras: It is the lifting of the free algebra functor [JSS15, Lemma 1], which is the left adjoint of the Eilenberg-Moore adjunction as given in Definition 2.3.41.

That being said, the general take-home message of this line of work is to not only look for theoretical advancements but to actually employ known results on concrete examples. In particular, whenever one is interested in determinization alike constructions, it could be worth to try lifting an adjunction (whenever that is possible) and see what the resulting construction does.

Last but not least we come back to behavioral pseudometrics. Since we have identified our coalgebraic framework of Chapter 5 as main conceptual contribution of this thesis, it is likely that the most promising line of future research should have its roots in this framework. As pointed out at the end of the chapter (see Section 5.9), there might be many ways not only to improve the current framework but maybe even generalize it further by allowing lattice valued metrics. Apart from that, the aforementioned take-home message still holds true: also this framework will benefit a lot from more examples.

A

Supplementary Material

A.1 Proofs and Calculations for Chapter 3

In this section we present all the missing proofs and detailed calculations for the results given in Chapter 3.

A.1.1 Determinization of Nondeterministic Automata

Let us first briefly check that indeed β_X^{-1} is the inverse of β_X : For any $S \in \mathcal{P}(A \times X + \mathbb{1})$ we calculate

$$\begin{aligned}\beta_X^{-1}(\beta_X(S)) &= \beta_X^{-1}(o_X(S), s_X(S)) \\ &= \{\checkmark \mid o_X(S) = 1\} \cup \bigcup_{a \in A} \{a\} \times s_X(S)(a) \\ &= \{\checkmark \mid \checkmark \in S\} \cup \{(a, x) \mid (a, x) \in S\} = S\end{aligned}$$

and for any $(o, s) \in \mathbb{2} \times (\mathcal{P}X)^A$ we have

$$\begin{aligned}\beta_X(\beta_X^{-1}((o, s))) &= \beta_X\left(\{\checkmark \mid o = 1\} \cup \bigcup_{a \in A} \{a\} \times s(a)\right) \\ &= \beta_X(\{\checkmark \mid o = 1\} \cup \{(a, x) \mid a \in A, x \in s(a)\}) \\ &= \left(o, \left(s' : A \rightarrow \mathcal{P}X, a \mapsto \bigcup_{\{(a, x) \mid x \in s(a)\}} \{x\}\right)\right) \\ &= (o, (s' : A \rightarrow \mathcal{P}X, a \mapsto s(a))) = (o, s) .\end{aligned}$$

Moreover, β and β^{-1} , are natural transformations: We consider the diagram

$$\begin{array}{ccc}
 \mathcal{P}(A \times X + \mathbb{1}) & \xrightarrow{\beta_X} & 2 \times (\mathcal{P}X)^A \\
 \downarrow \mathcal{P}(A \times f + \mathbb{1}) & \beta_X^{-1} & \downarrow 2 \times f[\cdot]^A \\
 \mathcal{P}(A \times Y + \mathbb{1}) & \xrightarrow{\beta_Y} & 2 \times (\mathcal{P}Y)^A \\
 & \beta_Y^{-1} &
 \end{array}$$

and remark that for any $S \in \mathcal{P}(A \times X + \mathbb{1})$ both $(\beta_Y \circ \mathcal{P}(A \times f + \mathbb{1}))(S)$ and $((2 \times f[\cdot]^A \circ \beta_X)(S))$ evaluate to the same tuple $(o_X(S), s_X(S))$ where

$$s_X(S): A \rightarrow \mathcal{P}X, \quad a \mapsto \bigcup_{(a,x) \in S} \{f(x)\}$$

and for $(o, s) \in 2 \times (\mathcal{P}X)^A$ we have

$$\begin{aligned}
 (\mathcal{P}(A \times f + \mathbb{1}) \circ \beta_X^{-1})(o, s) &= \{\checkmark \mid o = 1\} \cup \{(a, f(x)) \mid a \in A, x \in s(a)\} \\
 &= \{\checkmark \mid o = 1\} \cup \{(a, y) \mid a \in A, y \in (f \circ s)(a)\} \\
 &= (\beta_Y^{-1} \circ (2 \times f[\cdot]^A))(o, s)
 \end{aligned}$$

which completes the proof that β as defined by Equations (3.2.1) and (3.2.2) is a natural isomorphism.

For each set X we calculate $\alpha_X: 2 \times X^A \leftrightarrow A \times X + \mathbb{1}$ using Equation (3.1.6):

$$\begin{aligned}
 \alpha_X &= \varepsilon_{GLX} \circ L\beta_{LX}^{-1} \circ L\eta_X = \varepsilon_{A \times X + \mathbb{1}} \circ L\beta_X^{-1} \circ L(2 \times \eta_X^A) \\
 &= \varepsilon_{A \times X + \mathbb{1}} \circ L\beta_X^{-1} \circ \left\{ \left((o, s), (2 \times \eta_X^A)(o, s) \right) \mid o \in 2, s \in X^A \right\} \\
 &= \varepsilon_{A \times X + \mathbb{1}} \circ L\beta_X^{-1} \circ \left\{ \left((o, s), \left(o, (s': A \ni a \mapsto \{s(a)\} \in \mathcal{P}X) \right) \right) \mid \begin{array}{l} o \in 2, \\ s \in X^A \end{array} \right\} \\
 &= \varepsilon_{A \times X + \mathbb{1}} \circ \left\{ \left((o, s), \{\checkmark \mid o = 1\} \cup \bigcup_{a \in A} \{a\} \times s'(a) \right) \mid \begin{array}{l} o \in 2, \\ s \in X^A \end{array} \right\} \\
 &= \left\{ \left((1, s), \checkmark \right), \left((o, s), (a, s(a)) \right) \mid o \in 2, s \in X^A, a \in A \right\}
 \end{aligned}$$

which verifies Equation (3.2.4).

Now we proceed to calculate the lifted left adjoint using Equation (3.1.1). For any coalgebra $c: X \rightarrow 2 \times X^A$ we have

$$\bar{L}(c) = \alpha_X \circ Lc = \alpha_X \circ \{(x, c(x)) \mid x \in X\}$$

$$= \left\{ (x, \checkmark) \mid \begin{array}{l} x \in X, \\ \pi_1(c(x)) = 1 \end{array} \right\} \cup \left\{ (x, (a, \pi_2(c(x))(a))) \mid \begin{array}{l} x \in X, \\ a \in A \end{array} \right\}$$

which verifies Equation (3.2.5).

Analogously, we calculate the lifted right adjoint using Equation (3.1.2) where for any NA $d: Y \leftrightarrow A \times Y + \mathbb{1}$ the new DA $\bar{R}(d): \mathcal{P}Y \rightarrow \mathcal{2} \times (\mathcal{P}Y)^A$ is given by, for any set $Q \in \mathcal{P}Y$

$$\begin{aligned} \bar{R}(d)(Q) &= (\beta_Y \circ Rd)(Q) = \beta_Y(Rd(Q)) \\ &= \beta_Y(\{z \in A \times Y + \mathbb{1} \mid \exists q \in Q : (q, z) \in d\}) = (o, s) \end{aligned}$$

where $o = 1$ if there is a $q \in Q$ such that $(q, \checkmark) \in d$ and $o = 0$ else which verifies Equation (3.2.6) and $s: A \rightarrow \mathcal{P}Y, a \mapsto \{y \in Y \mid \exists q \in Q : (q, (a, y)) \in d\}$ which verifies Equation (3.2.7).

A.1.2 Codeterminization of Nondeterministic Automata

For each set X we calculate $\alpha_X: \mathcal{P}(A \times X + \mathbb{1}) \leftarrow A \times \mathcal{P}X + \mathbb{1}$ using Equation (3.1.6):

$$\begin{aligned} \alpha_X &= \varepsilon_{GLX} \circ L\beta_{LX}^{-1} \circ L\eta_X = \varepsilon_{A \times \mathcal{P}X + \mathbb{1}} \circ L\mathbb{1}_{A \times X + \mathbb{1}} \circ L(A \times \eta_X + \mathbb{1}) \\ &= \varepsilon_{A \times \mathcal{P}X + \mathbb{1}} \circ L(A \times \eta_X + \mathbb{1}) \end{aligned}$$

and evaluating this Set^{op} -arrow as a function yields:

$$\begin{aligned} \alpha_X(\checkmark) &= L(A \times \eta_X + \mathbb{1})(\varepsilon_{A \times \mathcal{P}X + \mathbb{1}}(\checkmark)) = L(A \times \eta_X + \mathbb{1})(\mathbb{1}) \\ &= \{z \in A \times \mathcal{P}X + \mathbb{1} \mid \exists z' \in \mathbb{1} : (z, z') \in (A \times \eta_X + \mathbb{1})\} \\ &= \{z \in A \times \mathcal{P}X + \mathbb{1} \mid (z, \checkmark) \in (A \times \eta_X + \mathbb{1})\} = \mathbb{1} \end{aligned}$$

and analogously for any $(a, S) \in A \times \mathcal{P}X$ we have

$$\begin{aligned} \alpha_X((a, S)) &= L(A \times \eta_X + \mathbb{1})(\varepsilon_{A \times \mathcal{P}X + \mathbb{1}}((a, S))) = L(A \times \eta_X + \mathbb{1})(\{(a, S)\}) \\ &= \{z \in A \times \mathcal{P}X + \mathbb{1} \mid \exists z' \in \{(a, S)\} : (z, z') \in (A \times \eta_X + \mathbb{1})\} \\ &= \{z \in A \times \mathcal{P}X + \mathbb{1} \mid (z, (a, S)) \in (A \times \eta_X + \mathbb{1})\} \\ &= \{(a, x) \in A \times \mathcal{P}X \mid x \in S\} = \{a\} \times S. \end{aligned}$$

We calculate the lifted left adjoint using Equation (3.1.1). For any $c: X \leftrightarrow A \times X + \mathbb{1}$ we obtain the Set^{op} -arrow $\bar{L}(c) = \alpha_X \circ Lc$ which, as a function is given by, for every $(a, S) \in A \times \mathcal{P}X$,

$$\bar{L}(c)((a, S)) = (Lc \circ \alpha_X)((a, S)) = Lc(\alpha_X((a, S))) = Lc(\{a\} \times S)$$

$$\begin{aligned} &= \{x \in X \mid \exists (a, y) \in \{a\} \times S : (x, (a, y)) \in c\} \\ &= \{x \in X \mid \exists y \in S : (x, (a, y)) \in c\} . \end{aligned}$$

Analogously we use Equation (3.1.2) to obtain the lifted right adjoint. For a coalgebra $d: Y \leftarrow A \times Y + \mathbb{1}$ we obtain

$$\begin{aligned} \bar{R}(d) &= \beta_Y \circ Rd = \{(y, \mathbb{1}) \in Y \times (A \times Y + \mathbb{1}) \mid d(\checkmark) = y\} \\ &\quad \cup \{(y, (a, y')) \in Y \times (A \times Y + \mathbb{1}) \mid d((a, y')) = y\} . \end{aligned}$$

A.1.3 Determinization of Deterministic Automata

For each set X we calculate the join preserving¹ function $\alpha_X: \mathcal{P}(2 \times X^A) \rightarrow 2 \times (\mathcal{P}X)^A$ using Equation (3.1.6)

$$\begin{aligned} \alpha_X &= \varepsilon_{GLX} \circ L\beta_{LX}^{-1} \circ LF\eta_X = \varepsilon_{(\mathcal{P}X, \sqcup)} \circ L\mathbb{1}_{\mathcal{P}X} \circ L(2 \times \eta_X^A) \\ &= \varepsilon_{(2 \times (\mathcal{P}X)^A, \sqcup)} \circ L(2 \times \eta_X^A) \end{aligned}$$

which for each $S \in \mathcal{P}(2 \times X^A)$ evaluates to

$$\alpha_X(S) = \left(\bigsqcup \{o \mid (o, s) \in S\}, \bigsqcup \{s \mid (o, s) \in S\} \right)$$

which is Equation (3.3.1). We calculate the lifted left adjoint using Equation (3.1.1). For any coalgebra $c: X \rightarrow 2 \times X^A$ we obtain a coalgebra $\bar{L}(c): \mathcal{P}X \rightarrow 2 \times (\mathcal{P}X)^A$ where for every $S \in \mathcal{P}X$ we have

$$\begin{aligned} \bar{L}(c)(S) &= (\alpha_X \circ Lc)(S) = \alpha_X(c[S]) \\ &= \left(\bigsqcup \{\pi_1(c(x)) \mid x \in S\}, \bigsqcup \{\pi_2(c(x)) \mid x \in S\} \right) \end{aligned}$$

Analogously we use Equation (3.1.2) to obtain the lifted right adjoint. For a coalgebra $d: (Y, \sqcup) \rightarrow (2 \times Y^A, \sqcup)$ we obtain

$$\bar{R}(d) = \beta_Y \circ Rd = Rd .$$

A.1.4 Codeterminization of Deterministic Join Automata

For this adjunction we will first give all the details of the base adjunction due to the fact that – to our knowledge – it is not standard construction.

¹It satisfies this property by construction!

Left adjoint

$$L: \mathbf{JSL} \rightarrow \mathbf{Set}^{\text{op}}, \quad L(X, \sqcup) = X, \quad L(f: (X, \sqcup) \rightarrow (Y, \sqcup)) = Lf: X \leftarrow Y$$

where $Lf(y) = \bigsqcup \{x \in X \mid f(x) \sqsubseteq y\}$.

Right adjoint

$$R: \mathbf{Set}^{\text{op}} \rightarrow \mathbf{JSL}, \quad RX = (\mathcal{P}X, \sqcup), \quad R(f: X \leftarrow Y) = f^{-1}[\cdot]: \mathcal{P}X \rightarrow \mathcal{P}Y$$

This is indeed a JSL-arrow due to the fact that the inverse image preserves arbitrary unions.

Unit

$$\eta_{(X, \sqcup)}: (X, \sqcup) \rightarrow (\mathcal{P}X, \sqcup), \quad x \mapsto \overline{\uparrow x} = \{x' \in X \mid x' \not\sqsupseteq x\}$$

Let us check that this is join-preserving. For binary joins we have

$$\begin{aligned} \eta_{(X, \sqcup)}(x \sqcup y) &= \{x' \in X \mid x' \not\sqsupseteq x \sqcup y\} = \overline{\{x' \in X \mid x' \sqsupseteq x \sqcup y\}} \\ &= \overline{\{x' \in X \mid x' \sqsupseteq x\} \cap \{x' \in X \mid x' \sqsupseteq y\}} \\ &= \{x' \in X \mid x' \not\sqsupseteq x\} \cup \{x' \in X \mid x' \not\sqsupseteq y\} = \eta_{(X, \sqcup)}(x) \cup \eta_{(X, \sqcup)}(y) \end{aligned}$$

which immediately can be generalized to arbitrary joins. In order to see that η is a natural transformation we calculate:

$$\begin{aligned} ((RLf) \circ \eta_{(X, \sqcup)})(x) &= (Lf)^{-1} [\overline{\uparrow x}] = \{y \in Y \mid (Lf)(y) \not\sqsupseteq x\} \\ &= \left\{ y \in Y \mid \bigsqcup \{x' \in X \mid y \sqsupseteq f(x')\} \not\sqsupseteq x \right\} \end{aligned}$$

and claim that

$$\{y \in Y \mid \bigsqcup \{x' \in X \mid y \sqsupseteq f(x')\} \not\sqsupseteq x\} = \{y \in Y \mid y \not\sqsupseteq f(x)\} = (\eta_{(Y, \sqcup)} \circ f)(x).$$

This is true because their complements are the same:

- ▷ Let $y \sqsupseteq f(x)$, then $x \in \{x' \in X \mid y \sqsupseteq f(x')\}$ and $\bigsqcup \{x' \in X \mid y \sqsupseteq f(x')\} \sqsupseteq x$.
- ▷ Conversely for $y \in \{y \in Y \mid \bigsqcup \{x' \in X \mid y \sqsupseteq f(x')\} \sqsupseteq x\}$ by join preservation and monotonicity we obtain

$$y \sqsupseteq \bigsqcup \{f(x') \mid y \sqsupseteq f(x')\} = f\left(\bigsqcup \{x' \in X \mid y \sqsupseteq f(x')\}\right) \sqsupseteq f(x).$$

Counit

This is simply $\varepsilon_X: \mathcal{P}X \leftarrow X, x \mapsto \overline{\{x\}}$ which is indeed a natural transformation (arrows to be read as functions):

$$\begin{aligned} (\text{LRf} \circ \varepsilon_Y)(y) &= L(f^{-1})(\overline{\{y\}}) = \bigsqcup \{S \in \mathcal{P}X \mid \overline{\{y\}} \supseteq f^{-1}[S]\} \\ &= \bigsqcup \{S \in \mathcal{P}X \mid \overline{\{y\}} \supseteq \{y' \in Y \mid f(y') \in S\}\} \\ &= \bigsqcup \{S \in \mathcal{P}X \mid f(y) \notin S\} = \overline{\{f(y)\}} = (\varepsilon_X \circ f)(y) \end{aligned}$$

Unit-Counit-Equations (2.3.3)

We have (arrows as functions)

$$\begin{aligned} (\text{L}\eta_{(X,\sqcup)} \circ \varepsilon_{\text{L}(X,\sqcup)})(x) &= \text{L}\eta_{(X,\sqcup)}(\overline{\{x\}}) = \bigsqcup \{x' \in X \mid \overline{\{x\}} \supseteq \eta_{(X,\sqcup)}(x')\} \\ &= \bigsqcup \{x' \in X \mid \overline{\{x\}} \supseteq \overline{\uparrow x'}\} = \bigsqcup \{x' \in X \mid \{x\} \subseteq \uparrow x'\} \\ &= \bigsqcup \{x' \in X \mid x \in \uparrow x'\} = \bigsqcup \{x' \in X \mid x \supseteq x'\} = x \end{aligned}$$

and in JSL:

$$\begin{aligned} (\text{R}\varepsilon_X \circ \eta_{\text{RX}})(S) &= \varepsilon_X^{-1} [\eta_{(\mathcal{P}X,\sqcup)}(S)] = \{x \in X \mid \varepsilon_X(x) \in \eta_{(\mathcal{P}X,\sqcup)}(S)\} \\ &= \{x \in X \mid \overline{\{x\}} \in \overline{\uparrow S}\} = \{x \in X \mid \overline{\{x\}} \not\supseteq S\} \\ &= \{x \in X \mid x \in S\} = S \end{aligned}$$

Lifting

We need a natural isomorphism $\beta: \text{RG} \Rightarrow \text{FR}$, i.e. for each set X we need a join-preserving function $\beta_X: (\mathcal{P}(A \times X + \mathbb{1}), \sqcup) \rightarrow (2 \times (\mathcal{P}X)^A, \sqcup)$. We take the bijective function given in Equation (3.3.6) from Section 3.2.2 which is:

$$\beta_X(S) = (\chi_S(\checkmark), (s: A \rightarrow \mathcal{P}X, s(a) = \{x \in X \mid (a, x) \in S\}))$$

In Section 3.2.2 we have already seen that this function is join-preserving. Using Equation (3.1.2) we calculate the lifted right adjoint:

$$\overline{\text{R}}(d: Y \leftarrow A \times Y + \mathbb{1}): (\mathcal{P}Y, \sqcup) \rightarrow (2 \times (\mathcal{P}Y)^A, \sqcup)$$

where we have

$$\overline{\text{R}}(d)(S) = \beta_Y \circ d^{-1}[S]$$

$$\begin{aligned}
&= \beta_Y(\{\checkmark \mid d(\checkmark) \in S\} \cup \{(a, y) \mid d((a, y)) \in S\}) \\
&= (\chi_S(d(\checkmark)), (s: A \rightarrow \mathcal{P}Y, s(a) = \{y \in Y \mid d((a, y)) \in S\}))
\end{aligned}$$

which is just the determinization of the automaton via the powerset construction. In order to obtain the lifted left adjoint we use Equation (3.1.6) to calculate $\alpha_{(X, \sqcup)} = \varepsilon_{GL(X, \sqcup)} \circ L\beta_{L(X, \sqcup)}^{-1} \circ LF\eta_{(X, \sqcup)}$ which is a Set^{op} -arrow (thus we have to reverse all arrows to calculate the function!). We calculate for arbitrary $(a, x) \in A \times X$:

$$\varepsilon_{A \times X + \mathbb{1}}(\checkmark) = \overline{\mathbb{1}} = A \times X, \quad \text{and} \quad \varepsilon_{A \times X + \mathbb{1}}((a, x)) = \overline{\{(a, x)\}}$$

and with that we continue

$$\begin{aligned}
&L\beta_{L(X, \sqcup)}^{-1}(A \times X) \\
&= \bigsqcup \left\{ (o, s) \in 2 \times (\mathcal{P}X)^A \mid A \times X \supseteq \beta_{L(X, \sqcup)}^{-1}((o, s)) \right\} \\
&= \bigsqcup \left\{ (o, s) \in 2 \times (\mathcal{P}X)^A \mid o = 0 \right\} \\
&= (0, (s'_{\checkmark}: A \rightarrow \mathcal{P}X, a \mapsto X))
\end{aligned}$$

and for the other cases

$$\begin{aligned}
L\beta_{L(X, \sqcup)}^{-1}(\overline{\{(a, x)\}}) &= \bigsqcup \left\{ (o, s) \in 2 \times (\mathcal{P}X)^A \mid \overline{\{(a, x)\}} \supseteq \beta_{L(X, \sqcup)}^{-1}((o, s)) \right\} \\
&= \bigsqcup \left\{ (o, s) \in 2 \times (\mathcal{P}X)^A \mid (a, x) \notin \beta_{L(X, \sqcup)}^{-1}((o, s)) \right\} \\
&= \bigsqcup \left\{ (o, s) \in 2 \times (\mathcal{P}X)^A \mid x \notin s(a) \right\} \\
&= \left(1, \left(s'_{(a, x)}: A \rightarrow \mathcal{P}X, s'_{(a, x)}(a') = \begin{cases} \overline{\{x\}}, & a' = a \\ X, & \text{else} \end{cases} \right) \right).
\end{aligned}$$

Finally we plug in these results to obtain

$$\begin{aligned}
LF\eta_{(X, \sqcup)}((0, s'_{\checkmark})) &= \bigsqcup \left\{ (o, s) \in 2 \times X^A \mid (0, s'_{\checkmark}) \sqsupseteq (o, \eta_{(X, \sqcup)}^A(s)) \right\} \\
&= \bigsqcup \left\{ (o, s) \in 2 \times X^A \mid o = 0 \wedge s'_{\checkmark} \sqsupseteq \eta_{(X, \sqcup)}^A(s) \right\} \\
&= \left(0, \bigsqcup \left\{ s \in X^A \mid s'_{\checkmark} \sqsupseteq \eta_{(X, \sqcup)}^A(s) \right\} \right) \\
&= \left(0, \left(s_{\checkmark}: A \rightarrow X, s_{\checkmark}(a) = \bigsqcup \{x' \in X \mid s'_{\checkmark}(a) \sqsupseteq \eta_{(X, \sqcup)}(x')\} \right) \right) \\
&= \left(0, \left(s_{\checkmark}: A \rightarrow X, s_{\checkmark}(a) = \bigsqcup \{x' \in X \mid X \supseteq \overline{\uparrow x'}\} \right) \right) \\
&= (0, (s_{\checkmark}: A \rightarrow X, s_{\checkmark}(a) = \top))
\end{aligned}$$

and for all other cases we get Equation (3.3.6):

$$\begin{aligned}
 \text{LF}\eta_{(X, \sqcup)} \left((1, s'_{(a, x)}) \right) &= \bigsqcup \left\{ (o, s) \in 2 \times X^A \mid (1, s'_{(a, x)}) \sqsupseteq (\text{F}\eta_{(X, \sqcup)})((o, s)) \right\} \\
 &= \bigsqcup \left\{ (o, s) \in 2 \times X^A \mid (1, s'_{(a, x)}) \sqsupseteq (o, \eta_{(X, \sqcup)}^A(s)) \right\} \\
 &= \bigsqcup \left\{ (o, s) \in 2 \times X^A \mid s'_{(a, x)} \sqsupseteq \eta_{(X, \sqcup)}^A(s) \right\} \\
 &= \left(1, \bigsqcup \left\{ s \in X^A \mid s'_{(a, x)} \sqsupseteq \eta_{(X, \sqcup)}^A(s) \right\} \right) \\
 &= \left(1, \left(s_{(a, x)} : A \rightarrow X, s_{(a, x)}(a') = \bigsqcup \left\{ x' \in X \mid s'_{(a, x)}(a') \sqsupseteq \eta_{(X, \sqcup)}(x') \right\} \right) \right) \\
 &= \left(1, \left(s_{(a, x)} : A \rightarrow X, s_{(a, x)}(a') = \bigsqcup \left\{ x' \in X \mid s'_{(a, x)}(a') \sqsupseteq \overline{\uparrow x'} \right\} \right) \right) \\
 &= \left(1, \left(s_{(a, x)} : A \rightarrow X, s_{(a, x)}(a') = \begin{cases} \bigsqcup \left\{ x' \in X \mid \overline{\{x\}} \sqsupseteq \overline{\uparrow x'} \right\}, & a' = a \\ \bigsqcup \left\{ x' \in X \mid X \sqsupseteq \overline{\uparrow x'} \right\}, & a' \neq a \end{cases} \right) \right) \\
 &= \left(1, \left(s_{(a, x)} : A \rightarrow X, s_{(a, x)}(a') = \begin{cases} \bigsqcup \{x' \in X \mid \{x\} \subseteq \uparrow x'\}, & a' = a \\ \top, & a' \neq a \end{cases} \right) \right) \\
 &= \left(1, \left(s_{(a, x)} : A \rightarrow X, s_{(a, x)}(a') = \begin{cases} \bigsqcup \{x' \in X \mid x \sqsupseteq x'\}, & a' = a \\ \top, & a' \neq a \end{cases} \right) \right) \\
 &= \left(1, \left(s_{(a, x)} : A \rightarrow X, s_{(a, x)}(a') = \begin{cases} x, & a' = a \\ \top, & a' \neq a \end{cases} \right) \right).
 \end{aligned}$$

With these results we can use Equation (3.1.1) to obtain the lifted left adjoint

$$\begin{aligned}
 \text{Lc}((1, s_{(a, x)})) &= \bigsqcup \{x' \in X \mid (1, s_{(a, x)}) \sqsupseteq c(x')\} \\
 &= \bigsqcup \{x' \in X \mid s_{(a, x)} \sqsupseteq \pi_2(c(x'))\} \\
 &= \bigsqcup \{x' \in X \mid \forall a' \in A : s_{(a, x)}(a') \sqsupseteq \pi_2(c(x'))(a')\} \\
 &= \bigsqcup \{x' \in X \mid s_{(a, x)}(a) \sqsupseteq s_{c(x')}(a)\} \\
 &= \bigsqcup \{x' \in X \mid x \sqsupseteq \pi_2(c(x'))(a)\}
 \end{aligned}$$

which is the supremum of all such x' whose a -successors are less or equal to x . Moreover, we obtain

$$\begin{aligned}
 \text{Lc}((0, s'_0)) &= \bigsqcup \{x' \in X \mid (0, s'_0) \sqsupseteq c(x')\} \\
 &= \bigsqcup \{x' \in X \mid (0, \top) \sqsupseteq c(x')\} \\
 &= \bigsqcup \{x' \in X \mid \pi_1(c(x')) = 0\}
 \end{aligned}$$

which is the supremum of all non-final states.

A.2 Borel-Measurability of the Trace Arrow Revisited

In Section 4.2.4 we used transfinite induction to show that the trace function is a Markov kernel. The following, alternative proof was suggested² to the author of this thesis by Ernst-Erich Doberkat after presenting the result on the Bellairs Workshop on Probability in 2014. It is much simpler and does not require any transfinite induction.

Let X be a set. We call a set $P \subseteq \mathcal{P}(X)$ a π -system on X , if it is non-empty and closed under finite intersections and a set $D \subseteq \mathcal{P}(X)$ a Dynkin system (or λ -system) on X if it contains X , is closed under complements and for any family $(A_n)_{n \in \mathbb{N}}$ of disjoint sets $A_n \in D$ also their union is in D [Els11, I. Def. 6.4].

Theorem A.2.1 (Dynkin's π - λ Theorem [Els11, I. Satz 6.7]) Let X be a set, P a π -system and D a Dynkin system on X such that $P \subseteq D$. Then $\sigma(P) \subseteq D$. \square

Using this we can prove the next result.

Lemma A.2.2 Let X, Y be sets, $P \subseteq \mathcal{P}(Y)$ a π -system containing Y and $k: X \times \sigma(P) \rightarrow [0, 1]$ a function such that $k(x, _)$ is a (sub-)probability measure for every $x \in X$. If $k(_, S)$ is measurable for every $S \in P$ then it is measurable for every $S \in \sigma(P)$ and thus a (Sub-)Markov kernel.

Proof. We aim at applying the π - λ theorem. We define the set

$$D := \{S \subseteq Y \mid x \mapsto k(x, S) \text{ is measurable}\}$$

and observe that we certainly have $P \subseteq D$. We proceed by showing that D is a Dynkin system. We have $X \in P \subseteq D$ and thus $X \in D$. If $S \in D$ we also have $Y \setminus S \in D$ because $x \mapsto k(x, Y \setminus S) = 1 - k(x, S)$ is measurable as difference of two measurable functions. Finally, for a countable family $(A_n)_{n \in \mathbb{N}}$ of disjoint sets $A_n \in D$ we have

$$k\left(x, \bigcup_{n \in \mathbb{N}} A_n\right) = \sum_{n \in \mathbb{N}} k(x, A_n) = \sup_{N \in \mathbb{N}} \sum_{1 \leq n \leq N} k(x, A_n)$$

which is measurable because it is the supremum of a family of measurable functions (which are themselves measurable because they are the finite sum of measurable functions). Thus D is a Dynkin system, so by the π - λ theorem we conclude $\sigma(P) \subseteq D$ which yields measurability for every $S \in \sigma(P)$. \square

²The presented version presented is based on some short proof sketches.

In order to employ this result to our trace function, we recall that by Theorem 4.2.12 $\text{tr}(x)$ is a (sub-)probability measure and by Lemma 4.2.19 for every $S \in \mathcal{S}_\diamond$ the function $x \mapsto \text{tr}(x)(S)$ is Borel-measurable. Now, since for each $\diamond \in \{*, \omega, \infty\}$ the sets \mathcal{S}_\diamond are semirings and thus π -systems the above Lemma A.2.2 yields the statement of Theorem 4.2.25, i.e., that $x \mapsto \text{tr}(x)(S)$ is Borel-measurable for every $S \in \sigma_{A^\diamond}(\mathcal{S}_\diamond)$.

A.3 Distributive Law for Probabilistic Automata

Here we prove that the distributive law $\lambda: \mathcal{D}_f([0, 1] \times _^A) \Rightarrow [0, 1] \times \mathcal{D}_f^A$ given in Lemma 5.8.5 (Page 214) is indeed a distributive law. We recall the definition of $\lambda_X = \langle o_X, s_X \rangle$ with

$$o_X(P) = \sum_{r \in [0, 1]} r \cdot P(r, X^A)$$

and

$$\begin{aligned} s_X(P): A &\rightarrow \mathcal{D}_f X, \\ s_X(P)(a)(x) &= \sum_{s \in X^A, s(a)=x} P([0, 1], s) = P\left([0, 1], \{s \in X^A \mid s(a) = x\}\right) \end{aligned}$$

for all sets X and all distributions $P: [0, 1] \times X^A \rightarrow [0, 1]$.

The proof that this is an \mathcal{EM} -law is carried out in the three following lemmas using just the definition of an \mathcal{EM} -law given in Definition 2.3.43 (Page 46).

Lemma A.3.1 λ as defined above is a natural transformation.

Proof. We have to show commutativity of the following diagram:

$$\begin{array}{ccc} \mathcal{D}_f([0, 1] \times X^A) & \xrightarrow{\lambda_X = \langle o_X, s_X \rangle} & [0, 1] \times (\mathcal{D}_f X)^A \\ \mathcal{D}_f(\text{id}_{[0, 1]} \times f^A) \downarrow & & \downarrow \text{id}_{[0, 1]} \times (\mathcal{D}_f f)^A \\ \mathcal{D}_f([0, 1] \times Y^A) & \xrightarrow{\lambda_Y = \langle o_Y, s_Y \rangle} & [0, 1] \times (\mathcal{D}_f Y)^A \end{array}$$

This is equivalent to the equality

$$\left(\text{id}_{[0, 1]} \times (\mathcal{D}_f f)^A\right) \circ \langle o_X, s_X \rangle = \langle o_Y, s_Y \rangle \circ \mathcal{D}_f(\text{id}_{[0, 1]} \times f^A)$$

which in turn is equivalent to the following two equalities

$$o_X = o_Y \circ \mathcal{D}_f(\text{id}_{[0,1]} \times f^A) \quad (\text{A.3.1})$$

$$(\mathcal{D}_f f)^A \circ s_X = s_Y \circ \mathcal{D}_f(\text{id}_{[0,1]} \times f^A) \quad (\text{A.3.2})$$

We will show them separately. Let $P \in \mathcal{D}_f([0,1] \times X^A)$. The right hand side of (A.3.1) evaluates to

$$\begin{aligned} o_Y \circ \mathcal{D}_f(\text{id}_{[0,1]} \times f^A)(P) &= o_Y\left(\mathcal{D}_f(\text{id}_{[0,1]} \times f^A)(P)\right) \\ &= \sum_{r \in [0,1]} r \cdot \mathcal{D}_f(\text{id}_{[0,1]} \times f^A)(P)(r, Y^A) = \sum_{r \in [0,1]} r \cdot \sum_{g \in Y^A} \mathcal{D}_f(\text{id}_{[0,1]} \times f^A)(P)(r, g) \\ &= \sum_{r \in [0,1]} r \cdot \sum_{g \in Y^A} P\left(r, \{h \in X^A \mid f \circ h = g\}\right) = \sum_{r \in [0,1]} r \cdot P(r, X^A) = o_X \end{aligned}$$

using for the second to last equality that for each $h \in X^A$ there is apparently a unique $g \in Y^A$ such that $f \circ h = g$, namely $g := f \circ h$. Thus we have shown (A.3.1).

In order to prove (A.3.2), we calculate both sides of the equality. For the left hand side we obtain for every $P \in \mathcal{D}_f([0,1] \times X^A)$, every $a \in A$ and every $y \in Y$

$$\begin{aligned} (\mathcal{D}_f f)^A \circ s_X(P)(a)(y) &= (\mathcal{D}_f f)(s_X(P)(a))(y) \\ &= s_X(P)(a)(\{x \in X \mid f(x) = y\}) \\ &= \sum_{x \in X, f(x)=y} s_X(P)(a)(x) \\ &= \sum_{x \in X, f(x)=y} \sum_{s \in X^A, s(a)=x} P([0,1], s) \\ &= \sum_{s \in X^A, f(s(a))=y} P([0,1], s) \\ &= \sum_{s \in X^A, f \circ s(a)=y} P([0,1], s). \end{aligned} \quad (\text{A.3.3})$$

For the right hand side of (A.3.2) we have

$$\begin{aligned} s_Y \circ \mathcal{D}_f(\text{id}_{[0,1]} \times f^A)(P)(a)(y) &= s_Y\left(\mathcal{D}_f(\text{id}_{[0,1]} \times f^A)(P)\right)(a)(y) \\ &= \mathcal{D}_f(\text{id}_{[0,1]} \times f^A)(P)\left([0,1], \{s' \in Y^A \mid s'(a) = y\}\right) \\ &= \sum_{s' \in Y^A, s'(a)=y} \mathcal{D}_f(\text{id}_{[0,1]} \times f^A)(P)([0,1], s) \end{aligned}$$

$$\begin{aligned}
 &= \sum_{s' \in Y^A, s'(a)=y} P([0, 1], \{s \in X^A \mid f \circ s = s'\}) \\
 &= \sum_{s' \in Y^A, s'(a)=y} \sum_{s \in X^A, f \circ s = s'} P([0, 1], s) \\
 &= \sum_{s \in X^A, f \circ s(a)=y} P([0, 1], s)
 \end{aligned}$$

which is the same as (A.3.3) so indeed (A.3.2) holds and thus λ is a natural transformation. \square

Lemma A.3.2 The diagram below commutes for all sets X .

$$\begin{array}{ccc}
 [0, 1] \times X^A & & \\
 \eta_{[0,1] \times X^A} \downarrow & \searrow \text{id}_{[0,1]} \times \eta_X^A & \\
 \mathcal{D}_f([0, 1] \times X^A) & \xrightarrow{\lambda_X = \langle o_X, s_X \rangle} & [0, 1] \times (\mathcal{D}_f X)^A
 \end{array}$$

Proof. Commutativity of the diagram is equivalent to

$$\langle o_X, s_X \rangle \circ \eta_{[0,1] \times X^A} = \text{id}_{[0,1]} \times \eta_X^A$$

which in turn is equivalent to requiring, for every $(r, s) \in [0, 1] \times X^A$,

$$o_X \circ \eta_{[0,1] \times X^A}(r, s) = \text{id}_{[0,1]}(r) = r, \quad (\text{A.3.4})$$

$$s_X \circ \eta_{[0,1] \times X^A}(r, s) = \eta_X^A(s). \quad (\text{A.3.5})$$

Showing (A.3.4) is straightforward: for every $(r, s) \in [0, 1] \times X^A$ we have

$$\begin{aligned}
 o_X \circ \eta_{[0,1] \times X^A}(r, s) &= o_X\left(\delta_{(r,s)}^{[0,1] \times X^A}\right) = \sum_{r' \in [0,1]} r' \cdot \delta_{(r,s)}^{[0,1] \times X^A}(r', X^A) \\
 &= r \cdot \delta_{(r,s)}^{[0,1] \times X^A}(r, s) = r
 \end{aligned}$$

where for every non-empty set Y and $y \in Y$ the function $\delta_y^Y: Y \rightarrow [0, 1]$ is the Dirac distribution, i.e., $\delta_y^Y(y') = 1$ if $y' = y$ and $\delta_y^Y(y') = 0$ else.

In order to show (A.3.5) we again compute both sides separately. For the left hand side we have, for all $(r, s) \in [0, 1] \times X^A$, all $a \in A$ and all $x \in X$,

$$s_X \circ \eta_{[0,1] \times X^A}(r, s)(a)(x) = s_X(\delta_{(r,s)}^{[0,1] \times X^A})(a)(x)$$

$$\begin{aligned}
 &= \delta_{(r,s)}^{[0,1] \times X^A} ([0,1], \{s' \in X^A \mid s'(a) = x\}) \\
 &= \begin{cases} 1, & \text{if } s(a) = x \\ 0, & \text{else} \end{cases}
 \end{aligned}$$

and for the right hand side

$$\eta_X^A(s)(a)(x) = \eta_X(s(a))(x) = \delta_{s(a)}^X(x) = \begin{cases} 1, & \text{if } s(a) = x \\ 0, & \text{else} \end{cases}$$

which completes our proof. \square

Lemma A.3.3 The diagram below commutes for all sets X .

$$\begin{array}{ccccc}
 \mathcal{D}_f^2([0,1] \times X^A) & \xrightarrow{\mathcal{D}_f \langle o_X, s_X \rangle} & \mathcal{D}_f([0,1] \times (\mathcal{D}_f X)^A) & \xrightarrow{\langle o_{\mathcal{D}_f X}, s_{\mathcal{D}_f X} \rangle} & [0,1] \times (\mathcal{D}_f^2 X)^A \\
 \downarrow \mu_{[0,1] \times X^A} & & & & \downarrow \text{id}_{[0,1]} \times \mu_X^A \\
 \mathcal{D}_f([0,1] \times X^A) & \xleftarrow{\langle o_X, s_X \rangle} & [0,1] \times (\mathcal{D}_f X)^A & &
 \end{array}$$

Proof. Commutativity of the diagram is equivalent to the two equalities

$$o_{\mathcal{D}_f X} \circ \mathcal{D}_f \langle o_X, s_X \rangle = o_X \circ \mu_{[0,1] \times X^A} \quad (\text{A.3.6})$$

$$\mu_X^A \circ s_{\mathcal{D}_f X} \circ \mathcal{D}_f \langle o_X, s_X \rangle = s_X \circ \mu_{[0,1] \times X^A} \quad (\text{A.3.7})$$

We compute the left hand side of (A.3.6) for $P \in \mathcal{D}_f^2([0,1] \times X^A)$ as

$$\begin{aligned}
 o_{\mathcal{D}_f X} \circ \mathcal{D}_f \langle o_X, s_X \rangle (P) &= o_{\mathcal{D}_f X}(\mathcal{D}_f \langle o_X, s_X \rangle (P)) \\
 &= \sum_{r \in [0,1]} r \cdot \mathcal{D}_f \langle o_X, s_X \rangle (P)(r, (\mathcal{D}_f X)^A) \\
 &= \sum_{r \in [0,1]} r \cdot \sum_{s \in (\mathcal{D}_f X)^A} \mathcal{D}_f \langle o_X, s_X \rangle (P)(r, s) \\
 &= \sum_{r \in [0,1]} r \cdot \sum_{s \in (\mathcal{D}_f X)^A} P\left(\left\{q \in \mathcal{D}_f([0,1] \times X^A) \mid o_X(q) = r, s_X(q) = s\right\}\right) \\
 &= \sum_{r \in [0,1]} r \cdot P\left(\left\{q \in \mathcal{D}_f([0,1] \times X^A) \mid o_X(q) = r\right\}\right)
 \end{aligned}$$

$$= \sum_{q \in \mathcal{D}_f([0,1] \times X^A)} o_X(P) \cdot P(q)$$

and the right hand side evaluates to

$$\begin{aligned} o_X \circ \mu_{[0,1] \times X^A}(P) &= \sum_{r \in [0,1]} r \cdot \mu_{[0,1] \times X^A}(P)(r, X^A) \\ &= \sum_{r \in [0,1]} r \cdot \sum_{s \in X^A} \mu_{[0,1] \times X^A}(P)(r, s) \\ &= \sum_{r \in [0,1]} r \cdot \sum_{s \in X^A} \sum_{q \in \mathcal{D}_f([0,1] \times X^A)} P(q) \cdot q(r, s) \\ &= \sum_{q \in \mathcal{D}_f([0,1] \times X^A)} P(q) \cdot \sum_{r \in [0,1]} r \cdot q(r, X^A) \\ &= \sum_{q \in \mathcal{D}_f([0,1] \times X^A)} P(q) \cdot o_X(q) \end{aligned}$$

so indeed (A.3.6) holds. We can rearrange the sums because they only contain non-negative values.

Also for (A.3.7) we first compute the left hand side for any $P \in \mathcal{D}_f^2([0, 1] \times X^A)$, any $a \in A$ and any $x \in X$

$$\begin{aligned} \mu_X^A \circ s_{\mathcal{D}_f X} \circ \mathcal{D}_f \langle o_X, s_X \rangle (P)(a)(x) &= \mu_X \left(s_{\mathcal{D}_f X} \left(\mathcal{D}_f \langle o_X, s_X \rangle (P) \right) (a) \right) (x) \\ &= \sum_{q \in \mathcal{D}_f X} q(x) \cdot s_{\mathcal{D}_f X} \left(\mathcal{D}_f \langle o_X, s_X \rangle (P) \right) (a)(q) \\ &= \sum_{q \in \mathcal{D}_f X} q(x) \cdot \mathcal{D}_f \langle o_X, s_X \rangle (P) \left([0, 1], \{s' \in (\mathcal{D}_f X)^A \mid s'(a) = q\} \right) \\ &= \sum_{s' \in (\mathcal{D}_f X)^A} s'(a)(x) \cdot \mathcal{D}_f \langle o_X, s_X \rangle (P) ([0, 1], s') \\ &= \sum_{s' \in (\mathcal{D}_f X)^A} s'(a)(x) \cdot \sum_{r \in [0,1]} \mathcal{D}_f \langle o_X, s_X \rangle (P)(r, s') \\ &= \sum_{s' \in (\mathcal{D}_f X)^A} s'(a)(x) \cdot \sum_{r \in [0,1]} P \left(\{q \in \mathcal{D}_f([0, 1] \times X^A) \mid o_X(q) = r, s_X(q) = s'\} \right) \\ &= \sum_{q \in \mathcal{D}_f([0,1] \times X^A)} s_X(q)(a)(x) \cdot P(q) \\ &= \sum_{q \in \mathcal{D}_f([0,1] \times X^A)} \sum_{s' \in X^A, s'(a)=x} \sum_{r \in [0,1]} q(r, s') \cdot P(q) \end{aligned}$$

and the right hand side evaluates to

$$\begin{aligned}
s_X \circ \mu_{[0,1] \times X^A}(P)(a)(x) &= s_X(\mu_{[0,1] \times X^A}(P))(a)(x) \\
&= \mu_{[0,1] \times X^A}(P)\left([0, 1], \{s' \in X^A \mid s'(a) = x\}\right) \\
&= \sum_{r \in [0,1]} \sum_{s' \in X^A, s'(a)=x} \mu_{[0,1] \times X^A}(P)(r, s') \\
&= \sum_{r \in [0,1]} \sum_{s' \in X^A, s'(a)=x} \sum_{q \in \mathcal{D}_f([0,1] \times X^A)} P(q) \cdot q(r, s)
\end{aligned}$$

which proves (A.3.7) and thus concludes the proof. \square

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List of Symbols

$-$	identity endofunctor on a category \mathcal{C} . 32
λ	the Lebesgue measure $\lambda: \mathcal{L} \rightarrow \overline{\mathbb{R}}$. 121
\otimes	product- σ -algebra or product measure. 91, 115
\odot	a measure similar to the product measure. 115
\checkmark	symbol for termination, the unique element of the singleton set $\mathbb{1}$. 17
χ_S	the characteristic function of the set S . 94
$\#$	the counting measure. 120
\diamond	a placeholder for the symbols $0, *, \omega, \infty$. 97
ε	the empty word. 20
\top	A chosen maximal element $0 < \top \leq \infty$. 135
$\mathbb{1}$	singleton set $\mathbb{1} = \{\checkmark\}$. 17
2	two element set, usually $2 = \{0, 1\}$. 17
ω	the first (smallest) infinite ordinal. 19
ω_1	the first (smallest) uncountable ordinal. 19
$[a, b]$	closed interval of extended real numbers. 17
$]a, b]$	half open interval of extended real numbers. 17
$]a, b[$	open interval of extended real numbers. 17
$[a, b[$	half open interval of extended real numbers. 17
A^*	the set of all finite words with letters from A . 7, 20
A^ω	the set of all infinite words with letters from A . 21
A^∞	the set of all words (finite and infinite) with letters from A . 21
\mathbb{A}	the class of all arrows of a category. 28
\mathfrak{B}	the Borel σ -algebra. 93

List of Symbols

bd_c	the bisimilarity pseudometric $\text{bd}_c: X^2 \rightarrow [0, \top]$ for a coalgebra $c: X \rightarrow FX$. 187
$[\mathfrak{C}, \mathfrak{D}]$	the functor (quasi-)category of functors from \mathfrak{C} to \mathfrak{D} and natural transformations. 40
$\mathfrak{C}(A, B)$	the class of arrows with domain A and codomain B of a category \mathfrak{C} . 28
Cat	the (large) category of small categories and functors. 33
$\text{CoAlg}(F)$	coalgebras of an endofunctor F . 52
$d^{\uparrow F}$	the Kantorovich pseudometric. 145
d^F	a lifted pseudometric. 144
$d^{\downarrow F}$	the Wasserstein pseudometric. 150
\mathcal{D}	the distribution functor. 32
$(d_1, \dots, d_n)^{\uparrow F}$	the Kantorovich pseudometric for a multifunctor $F: \text{Set}^n \rightarrow \text{Set}$. 172
$(d_1, \dots, d_n)^F$	a lifted pseudometric for a multifunctor $F: \text{Set}^n \rightarrow \text{Set}$. 171
$(d_1, \dots, d_n)^{\downarrow F}$	the Wasserstein pseudometric for a multifunctor $F: \text{Set}^n \rightarrow \text{Set}$. 173
\mathcal{D}_f	the finite-support probability distribution functor. 33
d_e	the Euclidean distance $d_e: [0, \top] \times [0, \top] \rightarrow [0, \top]$. 136
$\mathcal{EM}(T)$	the Eilenberg-Moore category of a monad (T, η, μ) . 46
ev_F	evaluation function for an endofunctor F on Set . 144
$\text{ev}_F * \text{ev}_G$	composition of evaluation functions yielding an evaluation function for FG . 194
\widetilde{F}	evaluation functor for an endofunctor F on Set or a multifunctor $F: \text{Set}^n \rightarrow \text{Set}$. 144
\overline{F}	lifting of a functor F to pseudometric spaces. 144
$f[A]$	the image of A for a function $f: X \rightarrow Y$ and $A \subseteq X$. 17

$f^{-1}[B]$	the preimage of B for a function $f: X \rightarrow Y$ and $B \subseteq Y$. 17
$[\![\cdot]\!]$	unique coalgebra homomorphism from a coalgebra c into the final coalgebra. 52
$\Gamma_F(t_1, t_2, \dots, t_n)$	the set of F -couplings of t_1, \dots, t_n for an endofunctor/a multifunctor F . 150
$\mathcal{I}(\mathcal{G})$	the closure of a set $\mathcal{G} \subseteq \mathcal{P}X$ under countable intersections. 101
$\text{Id}_{\mathcal{C}}$	identity endofunctor on a category \mathcal{C} . 32
Id_F	the identity natural transformation from a functor F to itself. 40
id_A	identity arrow of an object A in a category. 28
$\mathcal{Kl}(T)$	the Kleisli category of a monad (T, η, μ) . 44
\mathcal{L}	the Lebesgue σ -algebra. 120
$\lambda x. T$	lambda abstraction. 18
Meas	the category of measurable spaces and measurable functions. 91
\mathbf{O}	the object-class of a category, . 28
Ord	the class of all ordinals. 19
\mathbb{P}	the probability functor. 95
\mathcal{P}	the powerset functor. 32
\mathcal{P}_f	the finite powerset functor. 32
$\mathcal{P}X$	the powerclass of the class X . 17
$P_a(x, S)$	Markov kernel giving the transition probability of a PTS from state x with label a to set of states S . 97
PMet	the category of pseudometric spaces and non-expansive functions. 138
PTS	a probabilistic transition system. 97
\mathbb{R}	the set of real numbers. 17
\mathbb{R}_+	the set of non-negative real numbers. 17

List of Symbols

$\overline{\mathbb{R}}$	the set of extended real numbers. 17
$\overline{\mathbb{R}}_+$	the set of non-negative extended real numbers. 17
\mathcal{R}_\diamond	a function mapping ordinals to subsets of A^\diamond such that $\mathcal{R}_\diamond(\omega_1) = \sigma_{A^\diamond}(\mathcal{S}_\diamond)$. 101
\mathbf{Rel}	the category of sets and relations. 30
\mathbb{S}	the sub-probability functor. 95
\mathcal{S}_\diamond	a semiring of words where $\diamond \in \{0, *, \omega, \infty\}$. 99
\mathbf{Set}	the category of sets and functions. 29
\mathbf{SRel}	the category of stochastic relations. 96
td_c	the trace pseudometric $\mathrm{td}_c: X^2 \rightarrow [0, \top]$ for a coalgebra $c: X \rightarrow \mathbf{F}X$. 211
$\mathcal{U}(\mathcal{G})$	the closure of a set $\mathcal{G} \subseteq \mathcal{P}X$ under countable unions. 101
X/R	the set of all equivalence classes of an equivalence relation $R \subseteq X \times X$. 25
xRy	notation for $(x, y) \in R$ if $R \subseteq X \times Y$ is a binary relation. 17
$X \rightsquigarrow Y$	An arrow in a Kleisli category; corresponds to an arrow $X \rightarrow TY$ in the base category. 44
$X \leftrightarrow Y$	a binary relation from X to Y . 42

Index

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- \mathcal{KL} -law, 46
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